



# ***STIC Search Report***

## ***Biotech-Chem Library***

**STIC Database Tracking Number: 171184**

**TO: Deborah Lambkin**  
**Location: REM-5B09/5C18**  
**Art Unit: 1626**  
**November 22, 2005**

**Case Serial Number: 10/678331**

**From: P. Sheppard**  
**Location: Remsen Building**  
**Phone: (571) 272-2529**

**sheppard@uspto.gov**

### **Search Notes**

171184

Access DB# \_\_\_\_\_

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Deborah Lombum Examiner #: 71300 Date: 11/9/07  
Art Unit: 1626 Phone Number 302-0698 Serial Number: 10/678,331  
Mail Box and Bldg/Room Location: Rem5309 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

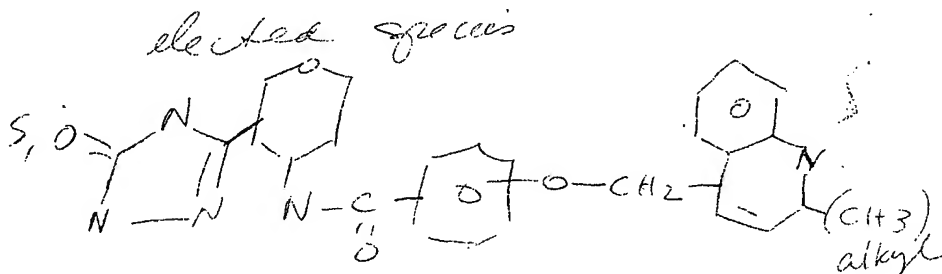
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: TRIAZOLONE & TRIAZOLETATION...

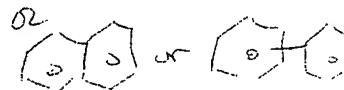
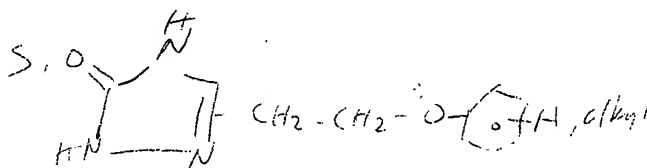
Inventors (please provide full names): B.W. King

Earliest Priority Filing Date: \_\_\_\_\_

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



*simplest compound*



*Empis looks too large to search, but  
if you would like to tackle it, ok.*

*Thank you*

## STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>5</u>	NA Sequence (#) _____	STN _____
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: _____	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: _____	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: _____	Other _____	Other (specify) _____

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(FILE 'REGISTRY' ENTERED AT 15:26:07 ON 22 NOV 2005)

L5 STR  
L7 48105 SEA SSS FUL L5  
L11 STR L9  
L12 39 SEA SUB=L7 SSS FUL L11

FILE 'HCAPLUS' ENTERED AT 15:31:56 ON 22 NOV 2005

L13 1 SEA ABB=ON PLU=ON L12  
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L19 195 SEA ABB=ON PLU=ON L18 NOT L12

FILE 'HCAPLUS' ENTERED AT 15:35:26 ON 22 NOV 2005

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L22 50 SEA ABB=ON PLU=ON L21 AND PD=<OCTOBER 7, 2003  
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D IBIB ABS HITSTR L22 1-50

#### FILE HCAPLUS

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FILE COVERS 1907 - 22 Nov 2005 VOL 143 ISS 22  
FILE LAST UPDATED: 21 Nov 2005 (20051121/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

#### FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 NOV 2005 HIGHEST RN 868586-21-4  
DICTIONARY FILE UPDATES: 21 NOV 2005 HIGHEST RN 868586-21-4

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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Lambkin 10\_678331- - History

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*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now      *
* available and contains the CA role and document type information.  *
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Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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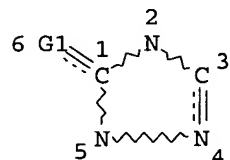
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New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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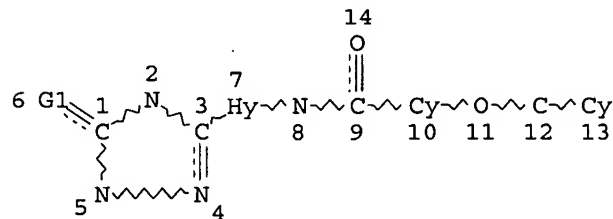
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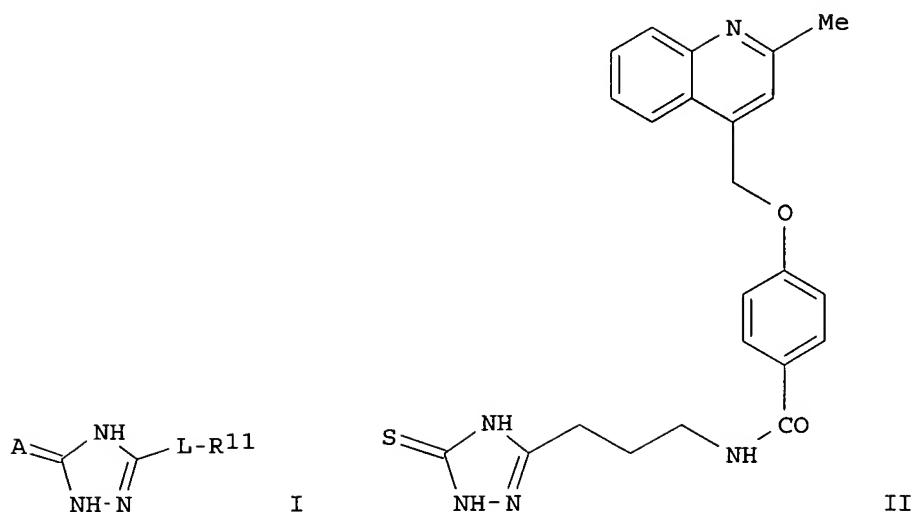


VAR G1=O/S  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 1  
 NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE  
 L7 48105 SEA FILE=REGISTRY SSS FUL L5  
 L11 STR





AB The present application describes novel hydantoin derivs. (shown as I; A = O, S; L-R11 represents a very large variety of substituents and is defined in the claims; e.g. II) or pharmaceutically acceptable salt or prodrug forms thereof, which are useful as inhibitors of matrix metalloproteinases (MMP), TNF- $\alpha$  converting enzyme (TACE), aggrecanase, or a combination thereof. Some examples of I exhibit  $K_i$ 's <10  $\mu$ M but individual data are not presented. Although the methods of preparation are not claimed, 37 example preps. are included. For example, II was prepared in 4 steps (100, 66, 73 and 82%, resp.) starting with condensation of Et 4-aminobutyrate hydrochloride with 4-(2-methylquinolin-4-ylmethoxy)benzoyl chloride hydrochloride followed by base hydrolysis to the acid, followed by hydrazide formation with thiosemicarbazide followed by cyclization.

IT 681284-32-2P 681284-35-5P 681284-36-6P  
 681284-41-3P 681284-46-8P 681284-50-4P  
 681284-62-8P 681284-63-9P 681284-67-3P  
 681284-68-4P 681284-70-8P 681284-71-9P  
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 681285-46-1P 681285-47-2P 681285-51-8P  
 681285-52-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of triazolone and triazolethione inhibitors of matrix metalloproteinases and/or TNF- $\alpha$  converting enzyme as anti-inflammatory agents)

RN 681284-32-2 HCAPLUS

CN Benzamide, N-[(3S,4R)-3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)tetrahydro-2H-pyran-4-yl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

Lambkin 10\_678331

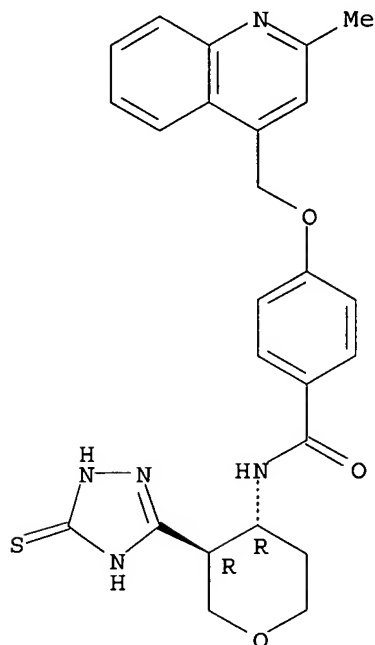
yl)tetrahydro-2H-pyran-4-yl]-4-[(2-methyl-4-quinolinyl)methoxy]-, rel-,  
trifluoroacetate (9CI) (CA INDEX NAME)

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CRN 681284-35-5

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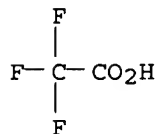
Relative stereochemistry.



CM 2

CRN 76-05-1

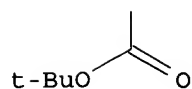
CMF C2 H F3 O2



RN 681284-41-3 HCAPLUS

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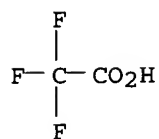
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



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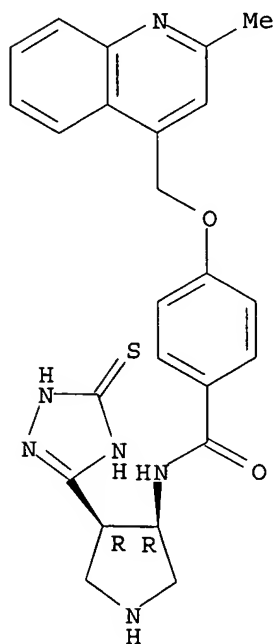
CN Benzamide, N-[(3R,4R)-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]-, rel-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

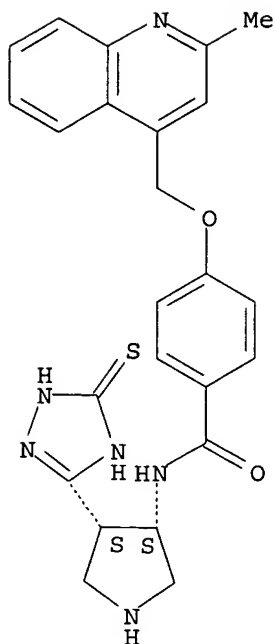
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Relative stereochemistry.



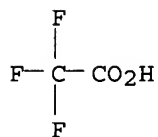




CM 2

CRN 76-05-1

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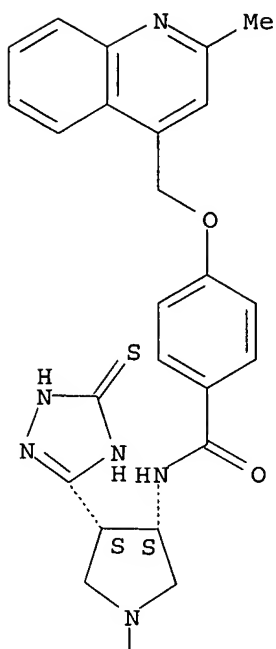


RN 681284-67-3 HCAPLUS

CN Benzamide, N-[(3S,4S)-1-acetyl-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



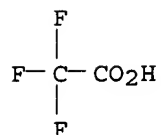
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CM 2

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CMF C2 H F3 O2

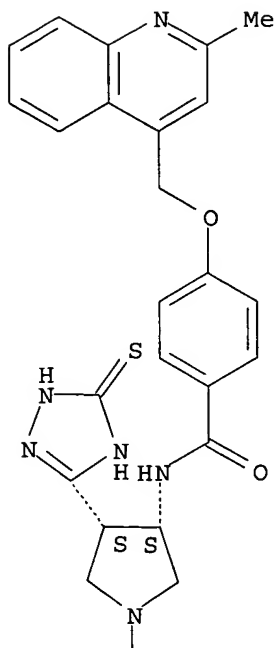


RN 681284-70-8 HCAPLUS

CN Benzamide, N-[(3S,4S)-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-1-propyl-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

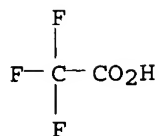


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Pr-n

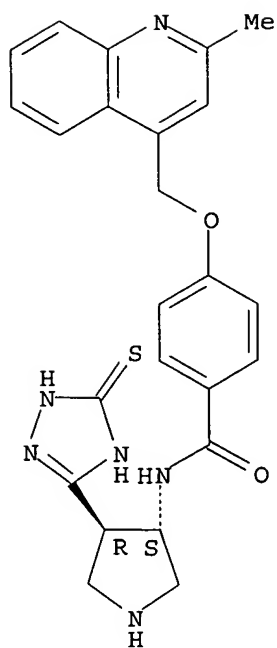
CM 2

CRN 76-05-1  
CMF C2 H F3 O2



RN 681284-80-0 HCAPLUS  
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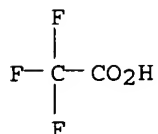
Relative stereochemistry.



CM 2

CRN 76-05-1

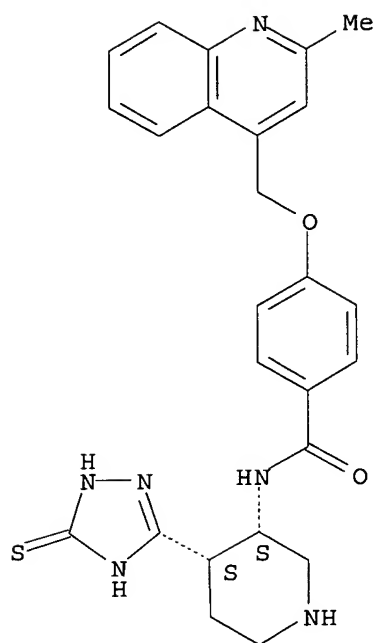
CMF C2 H F3 O2



RN 681284-91-3 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-, 1,1-dimethylethyl ester, (3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 681285-00-7 HCAPLUS  
 CN Benzamide, N-[(3S,4S)-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-piperidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]-, trifluoroacetate (9CI)  
 (CA INDEX NAME)

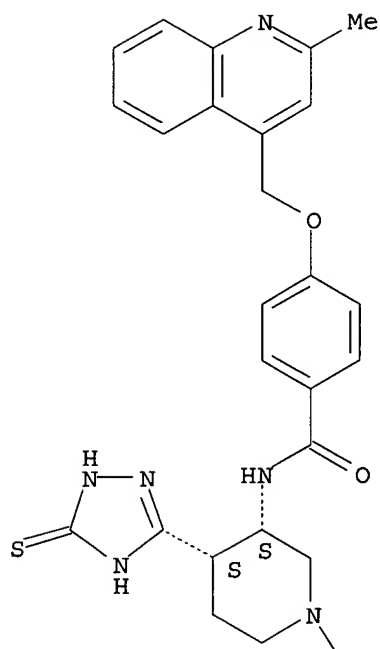
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CRN 681284-99-1

CMF C25 H26 N6 O2 S

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

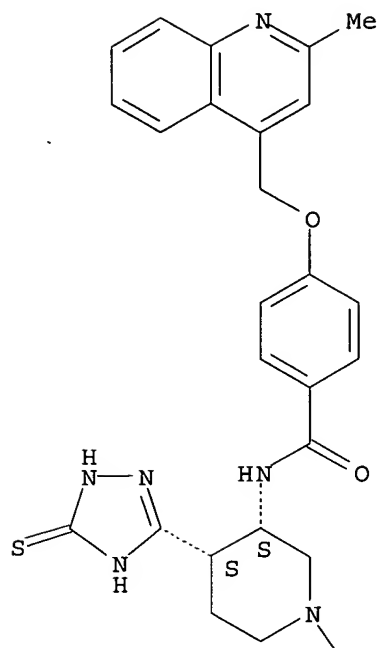


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CRN 681285-02-9  
 CMF C27 H28 N6 O3 S

Absolute stereochemistry.



Pr-n

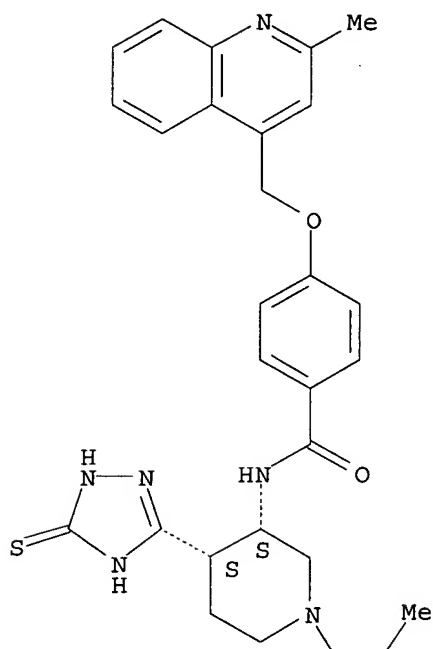
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CM 1

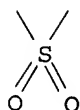
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 CMF C28 H32 N6 O2 S

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



RN 681285-17-6 HCAPLUS  
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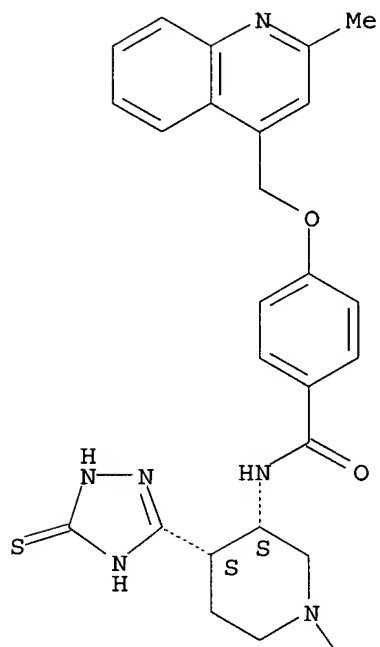
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Absolute stereochemistry.



PAGE 1-A



PAGE 2-A

Pr-i

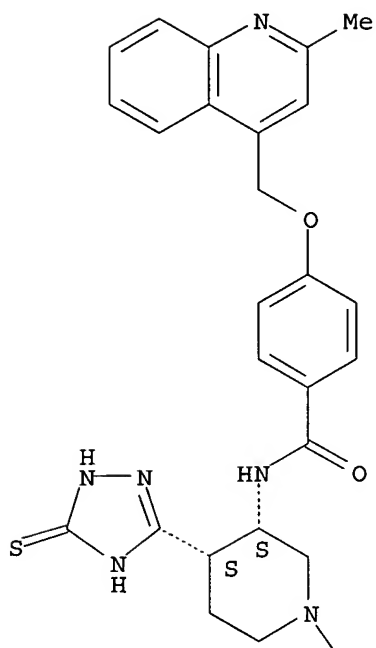
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CM 1

CRN 681285-21-2  
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Absolute stereochemistry.

PAGE 1-A



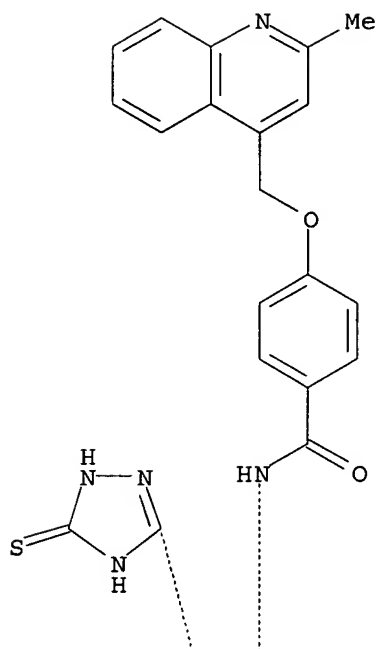
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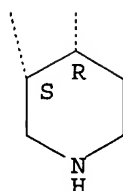
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 CN Benzamide, N-[(3S,4R)-3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4-piperidinyl]-4-[(2-methyl-4-quinolinyl)methoxy] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



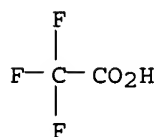
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CM 2

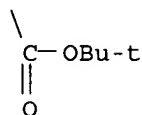
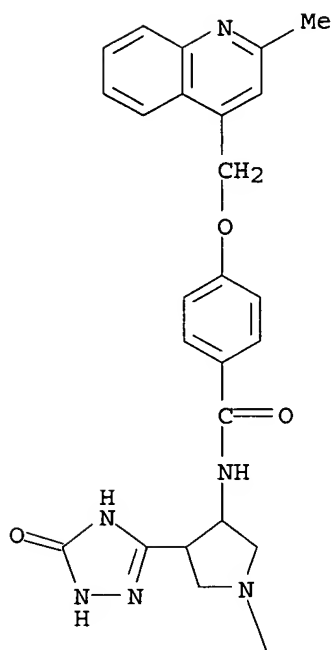
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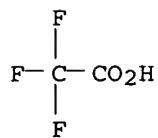
CN 1-Pyrrolidinecarboxylic acid, 3-(2,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl)-4-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



CM 2

CRN 76-05-1

CMF C2 H F3 O2



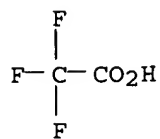
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CN Benzamide, N-[3-(2,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl)tetrahydro-2H-pyran-4-yl]-4-[(2-methyl-4-quinolyl)methoxy]- (9CI) (CA INDEX NAME)

CM 2

CRN 76-05-1

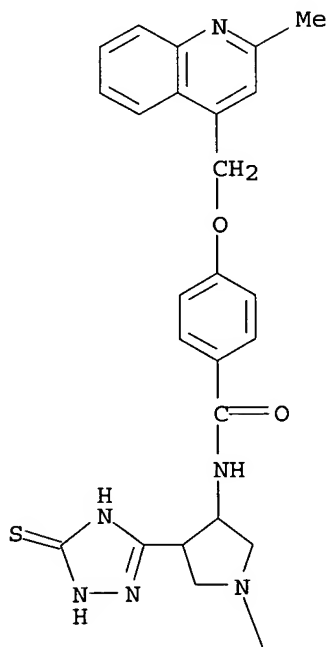
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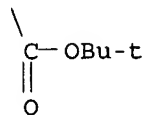
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CN 1-Pyrrolidinecarboxylic acid, 3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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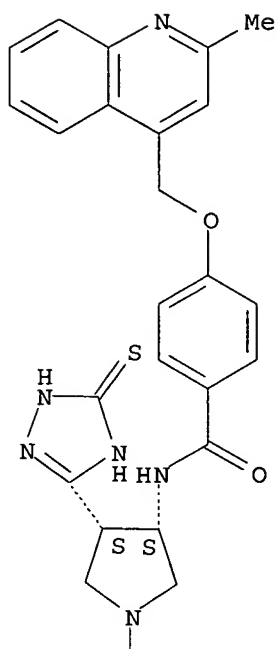
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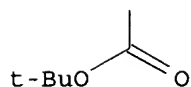
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PAGE 1-A

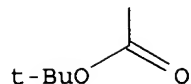


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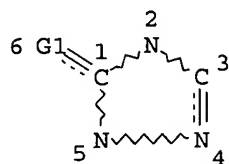
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 (CA INDEX NAME)

Absolute stereochemistry.



=> 0  
0 IS NOT A RECOGNIZED COMMAND

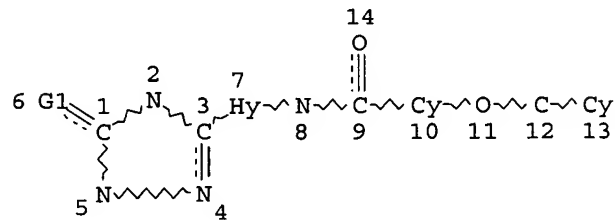
=> => d stat que  
L5 STR



VAR G1=O/S  
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RSPEC 1  
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE  
L7 48105 SEA FILE=REGISTRY SSS FUL L5  
L11 STR



VAR G1=O/S  
NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE  
L12 39 SEA FILE=REGISTRY SUB=L7 SSS FUL L11  
L13 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L12  
L17 STR

significant effects against *Bacillus subtilis* at MIC ranges of 0.5-1 µg/mL and moderate effects against *Staphylococcus aureus*.

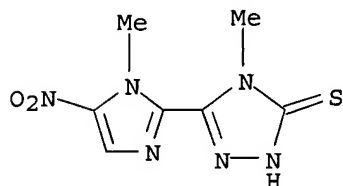
IT 590367-76-3P 590367-77-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and in vitro antimicrobial and antifungal evaluation of 5-(1-methyl-5-nitro-2-imidazolyl)-4H-1,2,4-triazoles)

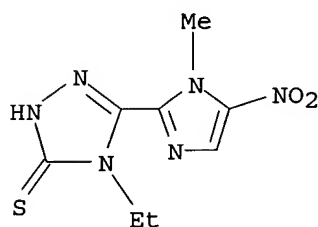
RN 590367-76-3 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 2,4-dihydro-4-methyl-5-(1-methyl-5-nitro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



RN 590367-77-4 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 4-ethyl-2,4-dihydro-5-(1-methyl-5-nitro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:5774 HCAPLUS

DOCUMENT NUMBER: 138:66658

TITLE: Novel nitrofuran-containing heterocyclic compounds and uses thereof

INVENTOR(S): Magee, Andrew S.; Roy, Aloka; Moe, Scott T.; Griffith, Jim P.; Ala, Paul J.; Ali, Janid; Clement, Jacob J.; Navia, Manuel

PATENT ASSIGNEE(S): Essential Therapeutics, Inc., USA; Pliva D.D.

SOURCE: PCT Int. Appl., 50 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

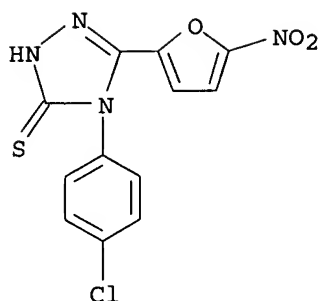
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000255	A1	20030103	WO 2002-US20387	20020625 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				





REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:217205 HCAPLUS

DOCUMENT NUMBER: 137:352962

TITLE: Synthesis of some new triazoles as potential antifungal agents

AUTHOR(S): Fahmy, Hesham T. Y.

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Alexandria, Alexandria, Egypt

SOURCE: Bollettino Chimico Farmaceutico (2001), 140(6), 422-427

CODEN: BCFAAI; ISSN: 0006-6648

PUBLISHER: Societa Editoriale Farmaceutica

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:352962

AB The rise in the incidence of fungal infections over the past two decades, particularly those caused by opportunistic pathogens in immune-compromised patients, has strengthened the need for new antifungal drugs. New triazole derivs. were synthesized and evaluated for their in-vitro antifungal activities against three species of fungi. Most of the prepared compds. showed good antifungal activity. Three compds. exhibited pronounced activity against *Cryptococcus neoformans* with MIC less than 12.5 g/mL.

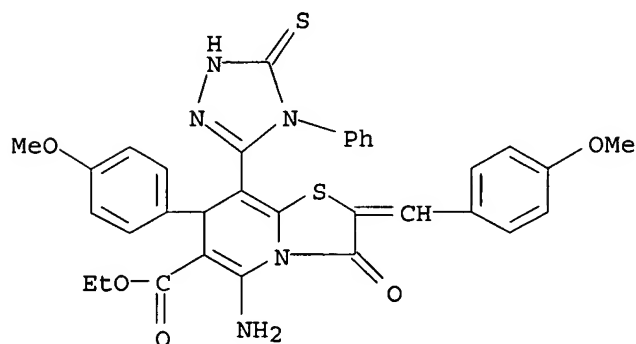
IT 474971-94-3P 474971-99-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation and antifungal activity of substituted triazoles)

RN 474971-94-3 HCAPLUS

CN 7H-Thiazolo[3,2-a]pyridine-6-carbonitrile, 5-amino-7-(4-chlorophenyl)-2-[(4-chlorophenyl)methylene]-8-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2,3-dihydro-3-oxo- (9CI) (CA INDEX NAME)

phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2,3-dihydro-7-(4-methoxyphenyl)-2-  
[(4-methoxyphenyl)methylene]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:693264 HCAPLUS

DOCUMENT NUMBER: 135:257269

TITLE: Preparation of N-heterocyclyl amide compounds as 5-HT  
antagonists

INVENTOR(S): Yamada, Akira; Tomishima, Masaki; Hayashida, Hisashi;  
Imanishi, Masashi; Spears, Glen W.; Ito, Kiyotaka;  
Takahashi, Fumie; Miyake, Hiroshi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 239 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

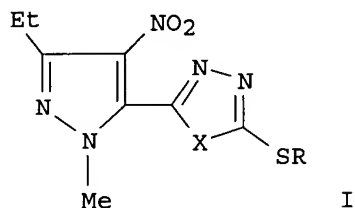
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001068585	A1	20010920	WO 2001-JP1993	20010313 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001041128	A5	20010924	AU 2001-41128	20010313 <--
EP 1264820	A1	20021211	EP 2001-912338	20010313 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004087798	A1	20040506	US 2002-221554	20021227
PRIORITY APPLN. INFO.:			JP 2000-70127	A 20000314
			JP 2000-305947	A 20001005
			WO 2001-JP1993	W 20010313

OTHER SOURCE(S): CASREACT 135:257269; MARPAT 135:257269

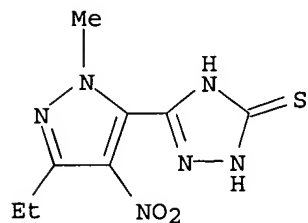
AB Amides compds. represented by the general formula R1-A-X-NHCO-Y-R2  
[wherein R1 is an optionally substituted heterocyclic group or optionally  
substituted phenyl; R2 is optionally substituted fused Ph, optionally

ACCESSION NUMBER: 2001:491585 HCAPLUS  
 DOCUMENT NUMBER: 135:210994  
 TITLE: Synthesis of pyrazolylheterocycles and their fungicidal activities  
 AUTHOR(S): Zhao, Wei-Guang; Chen, Han-Song; Li, Zheng-Ming; Han, Yu-Fen; Yan, Han; Lai, Jun-Ying; Wang, Su-Hua  
 CORPORATE SOURCE: Institute of Elemento-organic Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China  
 SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2001), 22(6), 939-942  
 CODEN: KTHPDM; ISSN: 0251-0790  
 PUBLISHER: Gaodeng Jiaoyu Chubanshe  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 OTHER SOURCE(S): CASREACT 135:210994  
 GI



AB Title compds. I (R = CH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>, CH<sub>2</sub>CH:CH<sub>2</sub>, CH<sub>2</sub>CO<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>, CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>; X = O, S, NH) were prepared from 1-methyl-3-ethyl-4-nitropyrzolylylcarboxylic acid. The structures of all new compds. were confirmed by <sup>1</sup>H NMR and elementary anal. Their fungicidal activity was evaluated against Rhizoctonia solani. Structure-activity relationships for the screened compds. were evaluated and discussed. It was found that some compds. showed a higher fungicidal activity and systematic activity.

IT 358641-26-6P 358641-27-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis and fungicidal activities of pyrazolylheterocycles)  
 RN 358641-26-6 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-(3-ethyl-1-methyl-4-nitro-1H-pyrazol-5-yl)-1,2-dihydro- (9CI) (CA INDEX NAME)



RN 358641-27-7 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-(3-ethyl-1-methyl-4-nitro-1H-pyrazol-5-yl)-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)

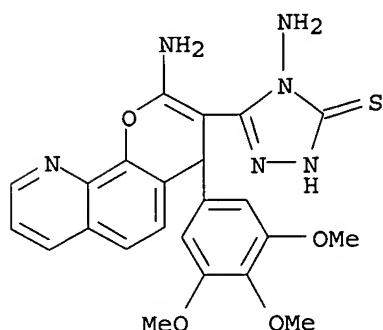
reaction of the carboxyhydrazide with Ph isothiocyanate, acetylacetone, and benzoylacetone resulted in the formation of II and III (R = Me, Ph), resp. Et carbazate as a typical mesophile reacted with I (R = COOEt) to afford a fused tetracyclic product, a triazepinopyranoquinoline, via cyclization of the initially formed hydrazide. Among sixteen compds. screened against E. coli and S. aureus, two compds. show a high order of antibacterial activity against both bacteria. IV is strongly potent against Staphylococcus aureus.

IT 389636-95-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and antibacterial activity of 4H-pyrano[3,2-h]quinolines and fused derivs.)

RN 389636-95-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 4-amino-5-[2-amino-4-(3,4,5-trimethoxyphenyl)-4H-pyrano[3,2-h]quinolin-3-yl]-2,4-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:334876 HCAPLUS

DOCUMENT NUMBER: 135:122486

TITLE: Heteroaromatization with ketene dithioacetals: Part I. Synthesis of some novel 5-amino-1-(1,3,4-thiadiazol-2-yl) and 1-(1,3,4-thiadiazin-2-yl)pyrazole-4-carbonitriles

AUTHOR(S): Hassan, Saber M.; Emam, Hussein A.; Abdelall, Mahmoud M.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar University, Cairo, 11884, Egypt

SOURCE: Journal of Chemical Research, Synopses (2000), (12), 544-545, 1301-1315  
CODEN: JRPSDC; ISSN: 0308-2342

PUBLISHER: Science Reviews Ltd.

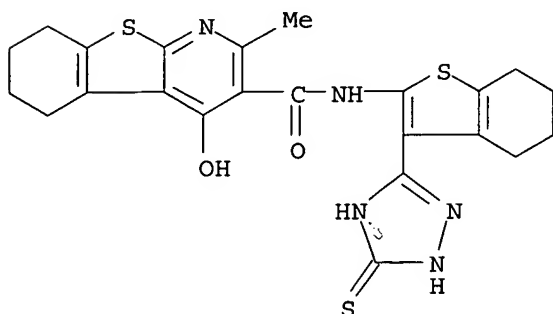
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:122486

AB 5-Amino-3-methylthio-1-(1,3,4-thiadiazol-2-yl) and 1-(1,3,4-thiadiazin-2-yl)pyrazole-4-carbonitriles were prepared from 5-aminopyrazoles using ketene dithioacetals as starting materials. For example, (MeS)<sub>2</sub>C:C(CN)<sub>2</sub> and (H<sub>2</sub>NNH)<sub>2</sub>C:S refluxed in EtOH gave 75% 1-(5-amino-4-cyano-3-methylthiopyrazol-1-yl)carbothiohydrazide (2a); 2a with PhCO<sub>2</sub>H and POCl<sub>3</sub> gave 65% 5-benzoylamino-3-methylthio-1-(5-phenyl-1,3,4-thiadiazol-2-yl)pyrazole-4-carbonitrile. 2A, chloroacetic acid and NaOAc in refluxing EtOH gave 66% 5-amino-3-methylthio-1-(5-oxo-1,3,4-thiadiazin-2-yl)pyrazole-

CN [1]Benzo[thieno[2,3-b]pyridine-3-carboxamide, N-[3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]-5,6,7,8-tetrahydro-4-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:631584 HCAPLUS

DOCUMENT NUMBER: 132:49927

TITLE: Synthesis, characterization and evaluation of the activity of ten mesoionic compounds against microorganisms

AUTHOR(S): De Athayde-Filho, Petronio Filgueiras; Miller, Joseph; Simas, Alfredo Mayall.; De Sena, Kesia Xisto da Fonseca Ribeiro; Chiappeta, Alda de Andrade

CORPORATE SOURCE: Departamento de Quimica, Universidade Federal Rural de Pernambuco, Recife-PE, 52.171-030, Brazil

SOURCE: Acta Farmaceutica Bonaerense (1999), 18(1), 17-22

CODEN: AFBODJ; ISSN: 0326-2383

PUBLISHER: Colegio de Farmaceuticos de la Provincia de Buenos Aires

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three mesoionic 1,3,4-thiadiazolium-2-thiolates and seven 1,3,4-triazolium-2-thiol chlorides have been synthesized and tested for activity against a range of microorganisms. The chemical structures were confirmed by elemental anal., IR, mass, <sup>1</sup>H and <sup>13</sup>C NMR spectrometry. The biol. tests indicate that the compds. have substantial activity against Gram-pos. and alc.-acid-resistant bacteria; moderate activity against yeasts and little activity against other fungi and are inactive against Gram-neg. bacteria.

IT 187875-14-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and bactericidal and fungicidal activity of thiadiazoliumthiolates and triazoliumthiol chlorides)

RN 187875-14-5 HCAPLUS

CN 1H-1,2,4-Triazolium, 4,5-dihydro-3-(5-nitro-2-furanyl)-2,4-diphenyl-5-thioxo-, chloride (9CI) (CA INDEX NAME)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

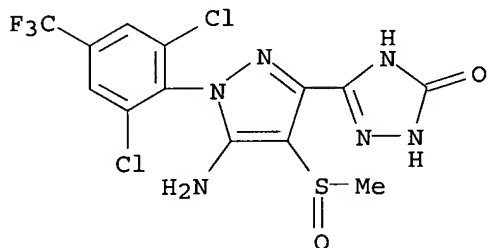
AB The title compds. [I; R1 = II-IV (R1a = H, alkyl, a lone pair of electrons; R1b = alkyl, aryl; X = O, NH, N(alkyl); Q = CR8R9, C(:Y), etc.; R8, R9 = H, alkyl, aryl, etc.; Y = O, S; Z = alkyl, aryl; W = H, alkyl, alkenyl, etc.; V = H, alkyl, CN, etc.); R2 = alkyl, haloalkyl, SOnR2a (R2a = alkyl, alkenyl, alkynyl, etc.); R3 = H, halo, alkyl, etc.; R4, R5, R7 = H, halo, alkyl; R6 = halo, haloalkyl, haloalkoxy, etc.; M = C(halo), C(Me), N, etc.], having pesticidal activity, were prepared Thus, reaction of 5-amino-1-(2,6-dichloro-4-trifluoromethylphenyl)-4-methylsulfinyl-3-[3-(1-amidoxime)]pyrazole (preparation given) with trifluoroacetic anhydride in dioxane afforded the title compound V which showed insecticidal activity in one or more of the evaluation methods (described in patent), with particularly good activity in the systemic tests.

IT 223582-94-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pesticidal 3-substituted arylpyrazoles)

RN 223582-94-3 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-[5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-1H-pyrazol-3-yl]-1,2-dihydro-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 11 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:424251 HCAPLUS

DOCUMENT NUMBER: 129:95500

TITLE: Preparation of 2-(1,2,4-triazol-3-ylthio)-, 2-(5-tetrazolylthio)-, 2-(1,3,4-thiadiazol-2-ylthio)thiazole compounds and methods of modulating signal transduction

INVENTOR(S): Tang, Peng C.; Ramphal, John Y.; Harris, G. Davis, Jr.; Nematalla, Asaad S.

PATENT ASSIGNEE(S): Sugen, Inc., USA

SOURCE: PCT Int. Appl., 175 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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cancer, colon cancer, or epidermoid cancer, and diabetes mellitus. Thus, 2-bromo-5-nitrothiazole was condensed with 4-[4-(4,5-dichloroimidazol-1-yl)phenyl]-2-mercaptopyrimidine at room temperature for 24 h to give the title compound, 4-(imidazolylphenyl)-2-(thiazolylthio)pyrimidine (II). In a phosphotyrosine enzyme linked immunosorbent assay, II inhibited dephosphorylation of phosphotyrosine residues on insulin receptor in NIH3T3 cells engineered to over-express the human insulin receptor (H25 cells) with EC50 (50% increase in the amount of phosphotyrosine over the control) of 3  $\mu$ M.

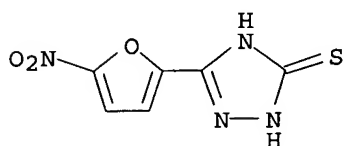
IT 57672-16-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of thiazole compds. modulating signal transduction as tyrosine phosphatase inhibitors for treatment of diseases)

RN 57672-16-9 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-5-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 12 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:391083 HCAPLUS

DOCUMENT NUMBER: 129:175593

TITLE: Synthesis, antifungal and antibacterial activity of substituted 1,2,4-triazoles

AUTHOR(S): Pourmorad, F.; Shafiee, A.

CORPORATE SOURCE: Department of Chemistry, Faculty of Pharmacy, The Medical Sciences University of Tehran, Tehran, Iran

SOURCE: Journal of Sciences, Islamic Republic of Iran (

1998), 9(1), 30-33

CODEN: JSIIEN; ISSN: 1016-1104

PUBLISHER: National Center for Scientific Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction of readily available 1-methyl-4-nitropyrrole-2-carboxylic acid with thionyl chloride afforded the corresponding carbonyl chloride. The reaction of the latter with thiosemicarbazides yielded 1-(1-methyl-4-nitropyrrole-2-carbonyl)thiosemicarbazides which cyclized in basic medium to 5-(1-methyl-4-nitropyrrole-2-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione derivs. Alkylation the latter and subsequent oxidation of (pyrrolyl)-1,2,4-triazoles. The antibacterial and antifungal activities of these against a number of microorganisms were determined Only two compds.

had moderate activity against *Aspergillus niger*.

IT 211626-82-3P 211626-83-4P 211626-84-5P

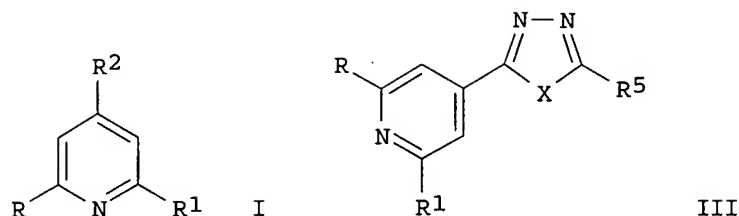
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antifungal and antibacterial activity of (pyrrolyl)-1,2,4-triazoles)

RN 211626-82-3 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 2,4-dihydro-5-(1-methyl-4-nitro-1H-pyrrol-2-yl)-4-phenyl- (9CI) (CA INDEX NAME)

GI



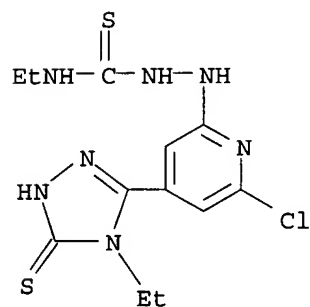
AB Condensation of pyridines I (R = R<sub>1</sub> = OH, R = Cl, R<sub>1</sub> = NHNH<sub>2</sub>, R<sub>2</sub> = CONHNH<sub>2</sub>) (II) with R<sub>3</sub>CHO (R<sub>3</sub> = Ph, 2,4-(OH)C<sub>6</sub>H<sub>3</sub>, 2-thienyl, 4-pyridyl, 4-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>) gave 35-87% I (R, R<sub>1</sub> = same as above, R<sub>2</sub> = CONHN:CHR<sub>3</sub>) and reactions of II with R<sub>4</sub>NCX (R<sub>4</sub> = Ph, Et; X = O, S) gave 31-89% I (R = Cl, OH; R<sub>1</sub> = OH, NHNHC(X)NHR<sub>4</sub>, R<sub>2</sub> = CONHNHC(X)NHR<sub>4</sub>), which cyclized to give 38-68% III (R = Cl, OH; R<sub>1</sub> = OH, NHNHC(X)NHR<sub>4</sub>, R<sub>5</sub> = XH, NHR<sub>4</sub>, X = O, S, NR<sub>4</sub>). Compds. I (R = R<sub>1</sub> = OH, R<sub>2</sub> = CONHN:CHPh) and III (R = R<sub>1</sub> = OH, R<sub>5</sub> = SH, X = NEt) were more effective as bactericides against *Bacillus subtilis* than ampicillin.

IT 197902-02-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation and microbicidal activity of)

RN 197902-02-6 HCAPLUS

CN Hydrazinecarbothioamide, 2-[6-chloro-4-(4-ethyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-2-pyridinyl]-N-ethyl- (9CI) (CA INDEX NAME)



IT 197901-99-8P 197902-00-4P 197902-03-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 197901-99-8 HCAPLUS

CN Hydrazinecarboxamide, 2-[6-chloro-4-(4-ethyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl)-2-pyridinyl]-N-ethyl- (9CI) (CA INDEX NAME)



CORPORATE SOURCE: Dep. Medicinal Chem., Fac. Pharmacy, Univ. Mansoura,  
Mansoura, 35516, Egypt  
SOURCE: Qatar University Science Journal (1994),  
14(Spec. Issue), 55-60  
CODEN: QUSJEV; ISSN: 1023-8948  
PUBLISHER: University of Qatar, Faculty of Science  
DOCUMENT TYPE: Journal  
LANGUAGE: English

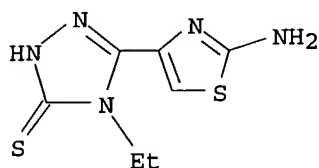
AB A series of thiazole derivs. bearing amino, acetamido or thioureido  
synthons at position 2 and thiosemicarbazone or 1,2,4-triazolethione  
moieties at position 4 have been synthesized and evaluated for their  
antimicrobial and antitumor activities. Some of the tested compds. proved  
to possess a remarkable antitumor antibiotic activity. The antimicrobial  
potency is found mainly to be against Gram pos. bacteria. The detailed  
synthesis, spectroscopic, and biol. data are reported.

IT 157521-62-5P 157521-63-6P 157521-64-7P  
157521-65-8P 157521-66-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and antimicrobial and antitumor activities of thiazoles)

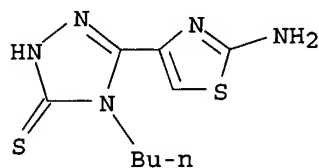
RN 157521-62-5 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-ethyl-2,4-dihydro-  
(9CI) (CA INDEX NAME)



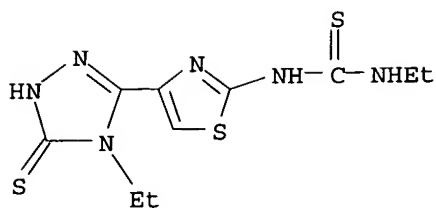
RN 157521-63-6 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-butyl-2,4-dihydro-  
(9CI) (CA INDEX NAME)



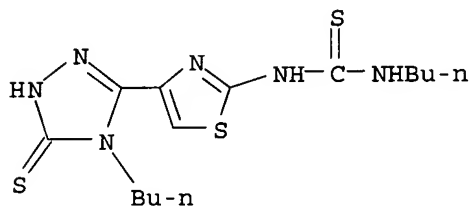
RN 157521-64-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-cyclohexyl-2,4-  
dihydro- (9CI) (CA INDEX NAME)



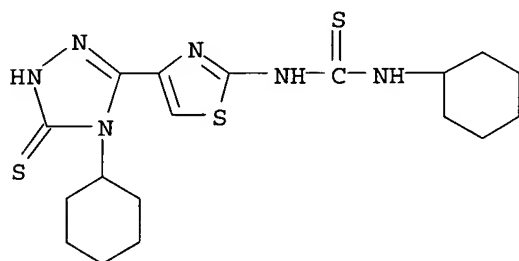
RN 157521-73-8 HCAPLUS

CN Thiourea, N-butyl-N'-[4-(4-butyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



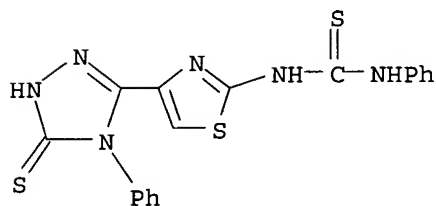
RN 157521-74-9 HCAPLUS

CN Thiourea, N-cyclohexyl-N'-[4-(4-cyclohexyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 157521-75-0 HCAPLUS

CN Thiourea, N-[4-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]-N'-phenyl- (9CI) (CA INDEX NAME)



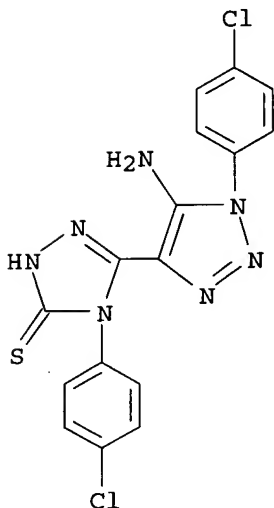
RN 157521-76-1 HCAPLUS

CN Thiourea, N-(4-fluorophenyl)-N'-[4-[4-(4-fluorophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl]-2-thiazolyl]- (9CI) (CA INDEX NAME)

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation of)

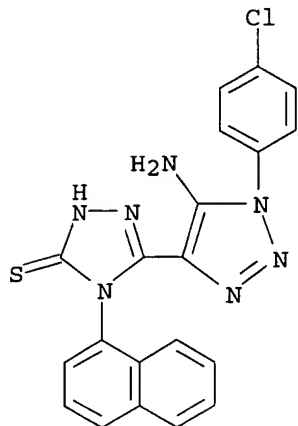
RN 188559-81-1 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-4-(4-chlorophenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)



RN 188559-85-5 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

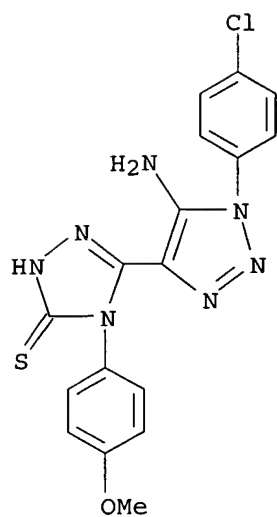


IT 188559-80-0P 188559-82-2P 188559-84-4P  
188559-86-6P 188559-87-7P 188559-88-8P  
188559-89-9P 188559-90-2P 188559-91-3P  
188559-92-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

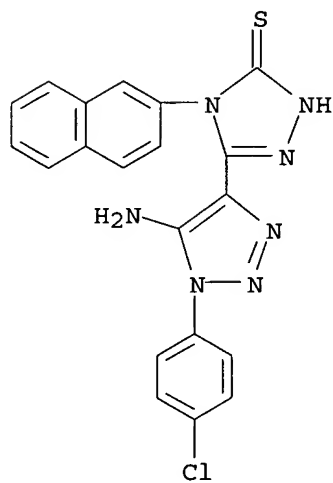
RN 188559-80-0 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)



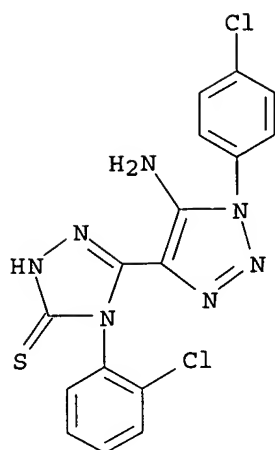
RN 188559-86-6 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



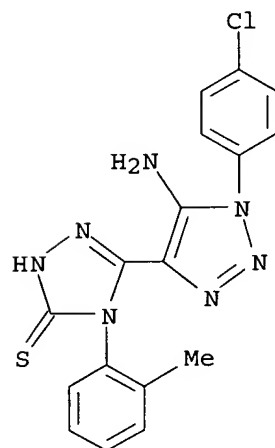
RN 188559-87-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-4-(4-ethoxyphenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)



RN 188559-90-2 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 188559-91-3 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(3-methylphenyl)- (9CI) (CA INDEX NAME)

PUBLISHER: Freund  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Mesoionic 1,4-diphenyl-5-(5-nitro-2-furanyl)-1,3,4-triazolium-2-thiolate was prepared as its hydrochloride by the reaction of 1,4-diphenylthiosemicarbazide with 5-nitro-2-furoyl chloride. The structure was confirmed by elemental anal., IR, mass, <sup>1</sup>H and <sup>13</sup>C NMR spectra. Pharmacol. tests in vitro showed that the compound possesses spasmolytic action in the guinea-pig trachea and the rat uterus, but not in the guinea-pig ileum.

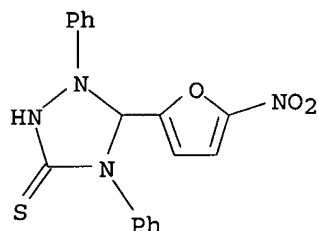
IT 187875-14-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and spasmolytic activity of diphenylnitrofuranyltriazoliumthiolate)

RN 187875-14-5 HCAPLUS

CN 1H-1,2,4-Triazolium, 4,5-dihydro-3-(5-nitro-2-furanyl)-2,4-diphenyl-5-thioxo-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L22 ANSWER 17 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:42600 HCAPLUS

DOCUMENT NUMBER: 126:186026

TITLE: Synthesis and biological studies of bis-heterocycles

AUTHOR(S): Kudari, S. M.; Beede, S. M.; Munera, Wahaja

CORPORATE SOURCE: Dep. Chem., Gulbarga Univ., Gulbarga, 585 106, India

SOURCE: Asian Journal of Chemistry (1997), 9(1), 20-26

CODEN: AJCHEW; ISSN: 0970-7077

PUBLISHER: Asian Journal of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

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RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 18 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

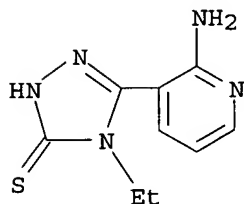
ACCESSION NUMBER: 1996:161585 HCAPLUS  
 DOCUMENT NUMBER: 124:220521  
 TITLE: Cytoprotection utilizing aryltriazol-3-thiones  
 INVENTOR(S): Connor, David T.; Plummer, Janet S.  
 PATENT ASSIGNEE(S): Warner-Lambert Co., USA  
 SOURCE: U.S., 7 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5489598	A	19960206	US 1994-255597	19940608 <--
PRIORITY APPLN. INFO.:			US 1994-255597	19940608
OTHER SOURCE(S): MARPAT 124:220521				

AB 5-Aryltriazol-3-thiones are useful for inhibiting adhesion of Mac-1 to the endothelium and thereby providing cytoprotection for diseases mediated by Mac-1 adhesion, such as nonsteroidal anti-inflammatory drug-induced gastritis, inflammatory bowel disease, and ulcerative colitis. The compds. were prepared and evaluated for inhibitory activity against Mac-1 adhesion in in vitro and in vivo models. For example, 5-(2-amino-5-chlorophenyl)-4-ethyl-2,4-dihydro-[1,2,4]triazol-3-thione inhibited the adhesion of Mac-1 to keyhole limpet hemocyanin-coated plates in vitro and prevented the aspirin-induced gastric damage in rats.

IT 174573-81-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (aryltriazol-3-thiones for inhibition of Mac-1 adhesion to endothelial cells for treatment of gastritis and colitis)

RN 174573-81-0 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-3-pyridinyl)-4-ethyl-2,4-dihydro-(9CI) (CA INDEX NAME)



L22 ANSWER 19 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:557485 HCAPLUS  
 DOCUMENT NUMBER: 121:157485  
 TITLE: Synthesis of some 2-(substituted thio)pyridines and thieno[2,3-b]pyridines  
 AUTHOR(S): Abdel-Monem, Maisa I.  
 CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, 71516, Egypt  
 SOURCE: Collection of Czechoslovak Chemical Communications (1994), 59(4), 978-86  
 CODEN: CCCCAK; ISSN: 0010-0765

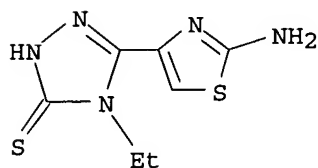
**157521-76-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and antibacterial and antitumor activities of, structure in relation to)

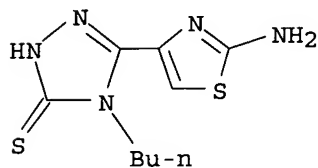
RN 157521-62-5 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-ethyl-2,4-dihydro-(9CI) (CA INDEX NAME)



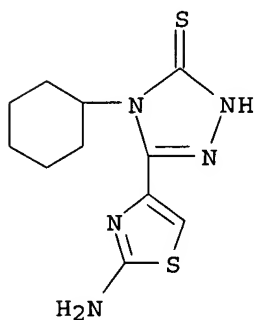
RN 157521-63-6 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-butyl-2,4-dihydro-(9CI) (CA INDEX NAME)



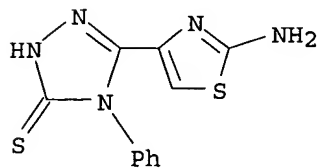
RN 157521-64-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-cyclohexyl-2,4-dihydro- (9CI) (CA INDEX NAME)

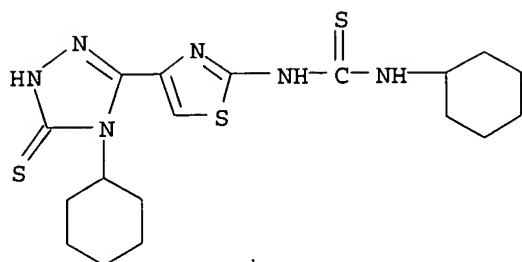


RN 157521-65-8 HCAPLUS

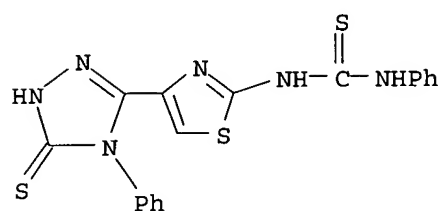
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-2,4-dihydro-4-phenyl-(9CI) (CA INDEX NAME)



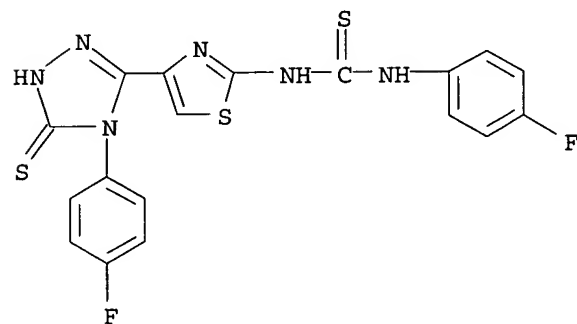




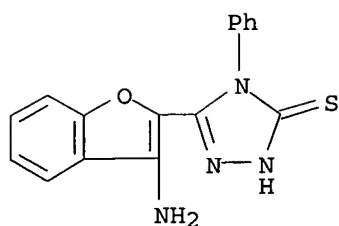
RN 157521-75-0 HCAPLUS  
 CN Thiourea, N-[4-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]-N'-phenyl- (9CI) (CA INDEX NAME)



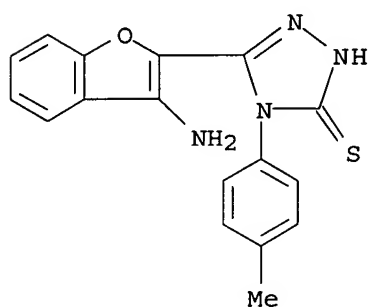
RN 157521-76-1 HCAPLUS  
 CN Thiourea, N-(4-fluorophenyl)-N'-[4-[4-(4-fluorophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl]-2-thiazolyl]- (9CI) (CA INDEX NAME)



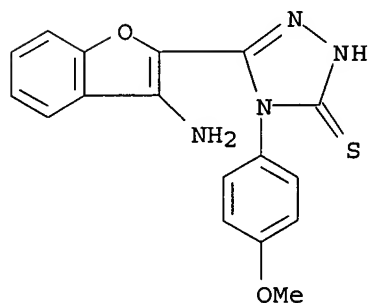
L22 ANSWER 21 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:22188 HCAPLUS  
 DOCUMENT NUMBER: 118:22188  
 TITLE: Synthesis of 1,3,4-oxadiazolyl, thiadiazolyl and 1,2,4-triazolyl-3-aminobenzofurans and related compounds  
 AUTHOR(S): Basavaraja, K. M.; Vaidya, V. P.; Sangapure, S. S.; Agasimundin, Y. S.  
 CORPORATE SOURCE: Dep. Chem., Gulbarga Univ., Gulbarga, 585 106, India  
 SOURCE: Indian Journal of Heterocyclic Chemistry (1992), 2(1), 35-40  
 CODEN: IJCHEI; ISSN: 0971-1627  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English



RN 144990-19-2 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-(3-amino-2-benzofuranyl)-2,4-dihydro-4-(4-methylphenyl)- (9CI) (CA INDEX NAME)

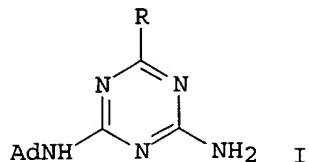


RN 144990-20-5 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-(3-amino-2-benzofuranyl)-2,4-dihydro-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 144990-21-6 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-(3-amino-2-benzofuranyl)-4-(4-chlorophenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)

OTHER SOURCE(S) : CASREACT 117:69834  
GI



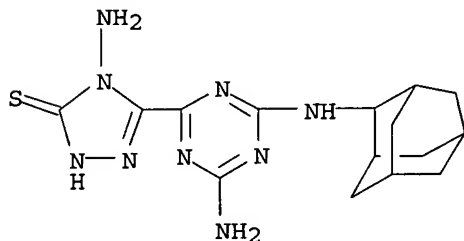
AB (Adamantylamino)triazines I [Ad = 2-adamantyl, R = CONHNHC(Z)NHR1 (Z = O, R1 = Pr, Ph; Z = S, R1 = alkyl, aryl, Ad)] and their cyclization products I (R = 4-R1-substituted-5-hydroxy(or mercapto)-1,2,4-triazol-3-yl) were prepared from hydrazide I (R = CONHNH2) and iso(thio)cyanates RNCZ. Cyclocondensation reactions were also carried out between the hydrazide and CS2 or CS2-N2H4-HCO2Et to give I (R = 5-mercapto-1,3,4-oxadiazol-2-yl) and I (R = 1,2,4-triazolo[5,4-b]-1,3,4-thiadiazol-3-yl), resp.

IT 142530-46-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclocondensation of, with formate)

RN 142530-46-9 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 4-amino-5-[4-amino-6-(tricyclo[3.3.1.3,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro- (9CI) (CA INDEX NAME)



IT 142530-35-6P 142530-36-7P 142530-37-8P

142530-38-9P 142530-39-0P 142530-40-3P

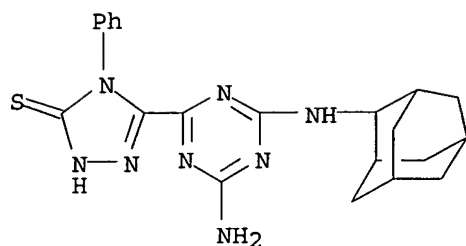
142530-41-4P 142530-42-5P 142530-43-6P

142530-44-7P

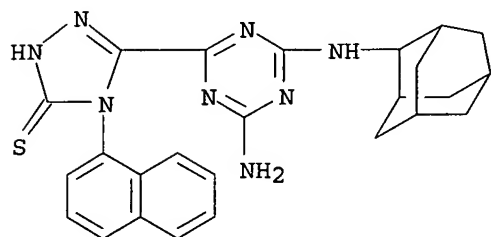
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 142530-35-6 HCAPLUS

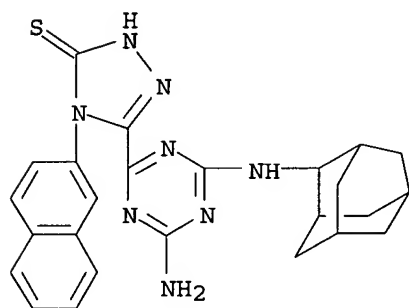
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.3,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)



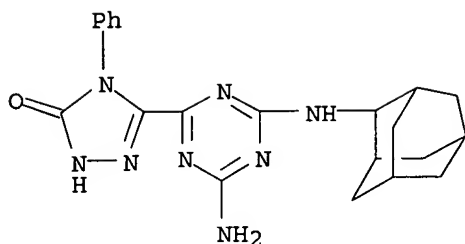
RN 142530-39-0 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.1<sup>3,7</sup>]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro-4-(1-naphthalenyl)- (9CI) (CA INDEX NAME)



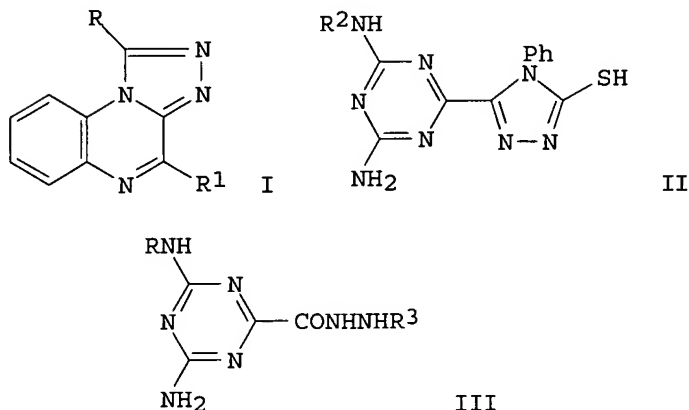
RN 142530-40-3 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.1<sup>3,7</sup>]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro-4-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 142530-41-4 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.1<sup>3,7</sup>]dec-2-ylamino)-1,3,5-triazin-2-yl]-4-(4-fluorophenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)



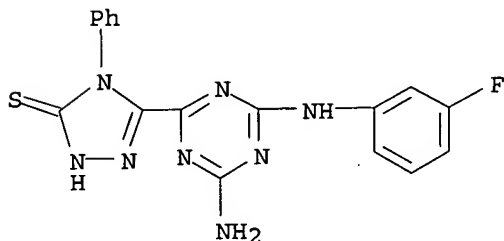
L22 ANSWER 23 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1992:59325 HCAPLUS  
 DOCUMENT NUMBER: 116:59325  
 TITLE: Synthesis and characterization of 1,2,4-triazolo[4,3-a]quinoxalines and 1,2,4-triazolo-s-triazines as potential antimicrobial agents  
 AUTHOR(S): El-Kerdawy, M.; Tantawy, A.; Gad, L. M.; Rady, E.  
 CORPORATE SOURCE: Fac. Pharm., Univ. Mansoura, Mansoura, Egypt  
 SOURCE: Zhonghua Yaoxue Zazhi (1991), 43(5), 355-64  
 CODEN: CYHCEX; ISSN: 1016-1015  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Several triazoloquinoxalines were synthesized via a series of reactions. Condensation of 2-chloro-3-hydrazinoquinoxaline with different aromatic aldehydes gave the corresponding hydrazones, which were directly cyclized to 4-chloro-1-aryl-1,2,4-triazolo[4,3-a]quinoxalines I (R = 4-BrC<sub>6</sub>H<sub>4</sub>, 2-ClC<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>; R<sub>1</sub> = Cl) in bromine/acetic acid. Subsequent displacement of the very reactive chloro substituent by a variety of nucleophiles was performed to yield 4-alkoxy and 4-substituted amino derivs. I (R<sub>1</sub> = OMe, OEt, morpholino, piperidino). Several s-triazole derivs. II (R<sub>2</sub> = 2-FC<sub>6</sub>H<sub>4</sub>, 2-MeSC<sub>6</sub>H<sub>4</sub>, 2-MeOC<sub>6</sub>H<sub>4</sub>) were prepared through the cyclization of the corresponding 4-amino-6-substituted anilino-s-triazine-2-carboxyhydrazides III (R<sub>3</sub> = H) using Ph isothiocyanate in alkaline medium, or by refluxing 1-phenyl-4-(4-amino-6-

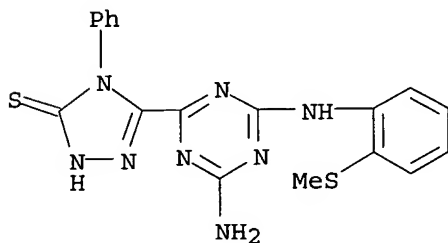
RN 138679-40-0 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-[(3-fluorophenyl)amino]-1,3,5-triazin-2-yl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)



RN 138679-41-1 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-[[2-(methylthio)phenyl]amino]-1,3,5-triazin-2-yl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)



L22 ANSWER 24 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:247213 HCAPLUS

DOCUMENT NUMBER: 114:247213

TITLE: Synthesis and spectrometric analysis of some new azopyrazole substituted 1,2,4-triazole-5-thiones

AUTHOR(S): Rollas, Sevim; Dogan, Nese; Ulgen, Mert; Ozger, Yasemin

CORPORATE SOURCE: Eczacihk Fak., Marmara Univ., Istanbul, Turk.

SOURCE: Marmara Universitesi Eczacilik Dergisi (1990

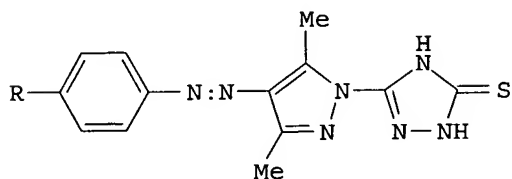
), 6(1), 41-7

CODEN: MUEDEZ; ISSN: 1011-3398

DOCUMENT TYPE: Journal

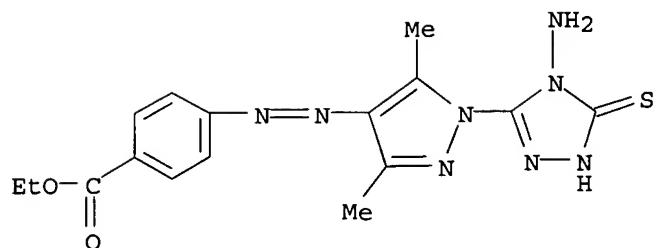
LANGUAGE: English

GI



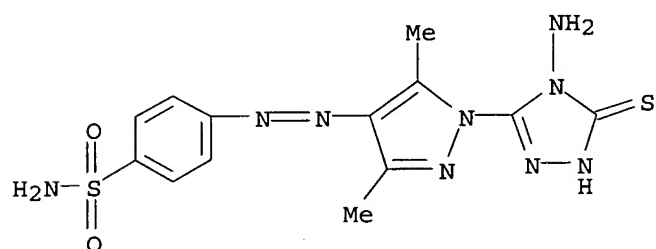
I

AB Title triazolethione I (R = H, NO<sub>2</sub>, CO<sub>2</sub>H, CO<sub>2</sub>Et, SO<sub>2</sub>NR<sub>1</sub>, R<sub>1</sub> = H, 4-methyl-2-pyrimidinyl, 4,6-dimethyl-2-pyrimidinyl) were prepared in 51-91%



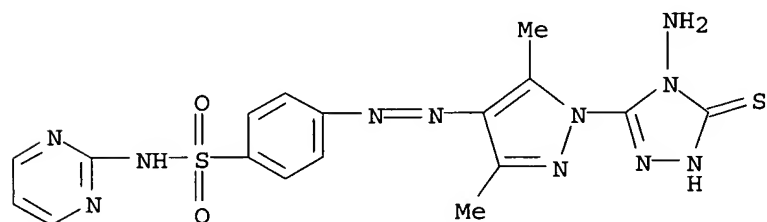
RN 133957-92-3 HCAPLUS

CN Benzenesulfonamide, 4-[[1-(4-amino-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3,5-dimethyl-1H-pyrazol-4-yl]azo]- (9CI) (CA INDEX NAME)



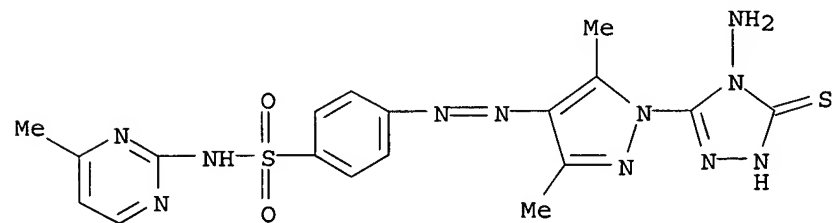
RN 133957-93-4 HCAPLUS

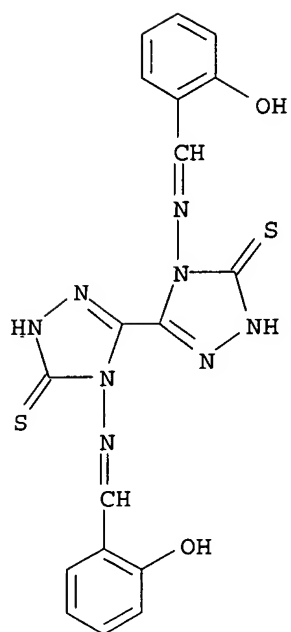
CN Benzenesulfonamide, 4-[[1-(4-amino-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3,5-dimethyl-1H-pyrazol-4-yl]azo]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)



RN 133957-94-5 HCAPLUS

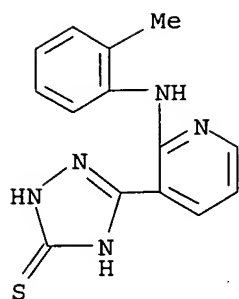
CN Benzenesulfonamide, 4-[[1-(4-amino-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3,5-dimethyl-1H-pyrazol-4-yl]azo]-N-(4-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)





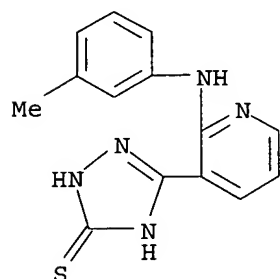
L22 ANSWER 26 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1989:192613 HCAPLUS  
 DOCUMENT NUMBER: 110:192613  
 TITLE: Some novel 2-substituted amino-3-heteroaryl-pyridines  
 as potential antimicrobial agents  
 AUTHOR(S): Abdel-Gawad, Mona; El-Telbany, F. A.; Badran, Mohga;  
 Ghoneim, Khadiga M.  
 CORPORATE SOURCE: Fac. Pharm., Cairo Univ., Cairo, Egypt  
 SOURCE: Egyptian Journal of Pharmaceutical Sciences (   
 1988), 29(1-4), 233-41  
 CODEN: EJPSBZ; ISSN: 0301-5068  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 110:192613  
 GI





RN 120137-36-2 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-5-[2-[(3-methylphenyl)amino]-3-pyridinyl]- (9CI) (CA INDEX NAME)



L22 ANSWER 27 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:6027 HCAPLUS

DOCUMENT NUMBER: 108:6027

TITLE: Preparation of alkyl 5-substituted-3-mercapto-4H-1,2,4-triazol-4-yl acetates as antiinflammatories and antibiotic intermediates

INVENTOR(S): Veverka, Miroslav; Marchalin, Miroslav

PATENT ASSIGNEE(S): Czech.

SOURCE: Czech., 5 pp.

CODEN: CZXXA9

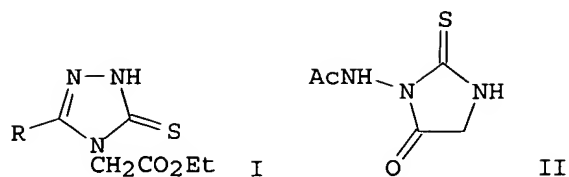
DOCUMENT TYPE: Patent

LANGUAGE: Slovak

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 234892	B1	19850416	CS 1984-882	19840207 <--
PRIORITY APPLN. INFO.:			CS 1984-882	19840207
OTHER SOURCE(S):	CASREACT	108:6027		
GI				



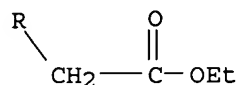
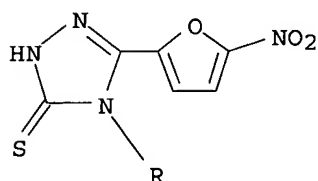
AB Et (3-substituted 5-thioxo-1,2,4-triazolin-4-yl)acetates I (R = e.g. H, Me, Ph, PhCH<sub>2</sub>, 2-thienyl) were prepared by addition-cyclization reaction of Et isothiocyanatoacetate with carboxylic acid hydrazides in the presence of NaOEt. Thermal cyclization of the adduct AcNHNHCSNHCH<sub>2</sub>CO<sub>2</sub>Et in DMF afforded 1-acetamido-2-thiohydantoin II. The effect of substituents on the cyclization course and the thione-thiol tautomerism are discussed.

IT 110167-69-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 110167-69-6 HCAPLUS

CN 4H-1,2,4-Triazole-4-acetic acid, 1,5-dihydro-3-(5-nitro-2-furanyl)-5-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



L22 ANSWER 29 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:608833 HCAPLUS

DOCUMENT NUMBER: 105:208833

TITLE: Oxidation of aldehyde semicarbazones with lead dioxide: application to the syntheses of 2-amino-1,3,4-oxadiazoles and 2,4-dihydro-1,2,4-triazol-3-ones

AUTHOR(S): Thu Huong Nguyen; Milcent, Rene; Barbier, Geo

CORPORATE SOURCE: Fac. Med., Univ. Paris, Paris, 75018, Fr.

SOURCE: Journal of Heterocyclic Chemistry (1985), 22(5), 1383-8

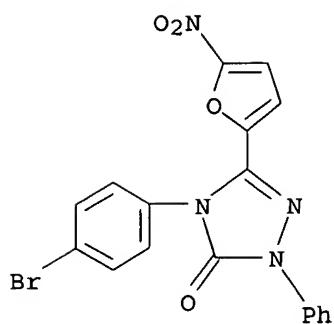
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

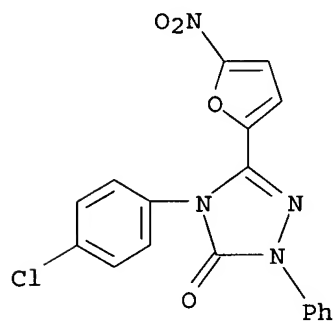
OTHER SOURCE(S): CASREACT 105:208833

GI



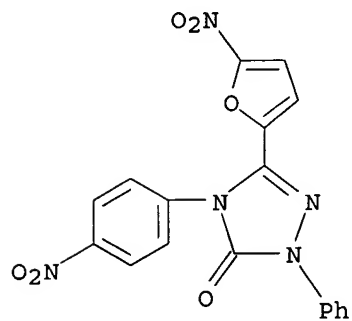
RN 104707-70-2 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-(4-chlorophenyl)-2,4-dihydro-5-(5-nitro-2-furanyl)-2-phenyl- (9CI) (CA INDEX NAME)



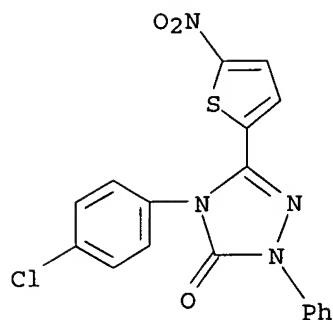
RN 104707-71-3 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-(5-nitro-2-furanyl)-4-(4-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)

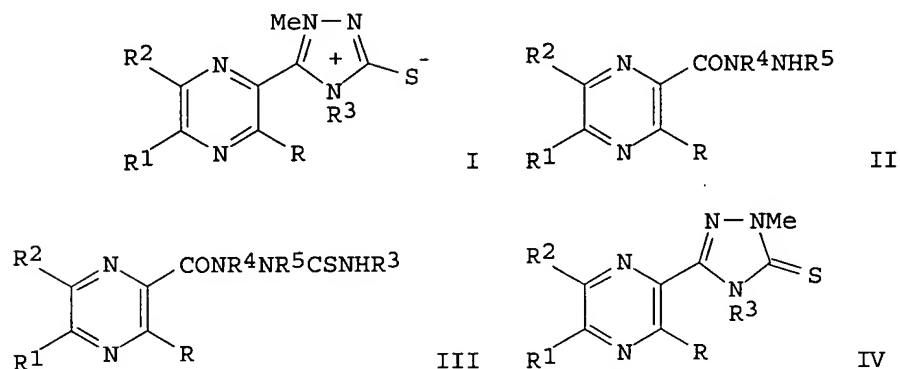


RN 104707-72-4 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-(5-nitro-2-thienyl)-2,4-diphenyl- (9CI) (CA INDEX NAME)

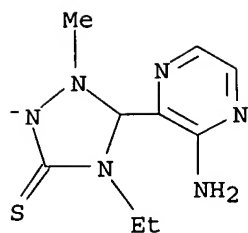


L22 ANSWER 30 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1982:68940 HCAPLUS  
 DOCUMENT NUMBER: 96:68940  
 TITLE: Synthesis of anhydro-3-mercapto-5-pyrazinyl-1,2,4-triazolium hydroxides  
 AUTHOR(S): Shutske, Gregory M.  
 CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc.,  
 Somerville, NJ, 08876, USA  
 SOURCE: Journal of Heterocyclic Chemistry (1981),  
 18(5), 1017-23  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 96:68940  
 GI



AB The synthesis of some novel anhydro-3-mercapto-5-pyrazinyl-1,2,4-triazolium hydroxides (I; R = H, NH<sub>2</sub>, NHAc; R<sub>1</sub> = H, NH<sub>2</sub>; R<sub>2</sub> = Et, H, Cl; R<sub>3</sub> = alkyl, aryl, etc.) is described. The appropriate 1-methylhydrazides II (R<sub>4</sub> = Me, R<sub>5</sub> = H) were condensed with R<sub>3</sub>NCS to give the thiosemicarbazides III which were cyclized to I under mildly basic conditions. A few 1,2,4-triazole-3-thiones IV were synthesized for comparison, starting with the 2-methylhydrazides (II; R<sub>4</sub> = H, R<sub>5</sub> = Me) and then carrying out analogous synthetic transformations.

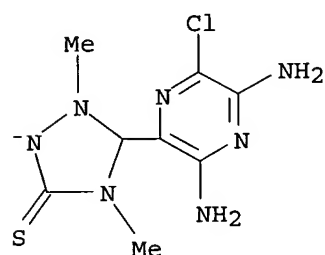
IT 79998-06-4P 79998-07-5P 79998-08-6P  
 79998-09-7P 79998-10-0P 79998-14-4P  
 79998-15-5P 79998-18-8P 79998-19-9P  
 79998-20-2P 80364-55-2P 80364-56-3P



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-10-0 HCAPLUS

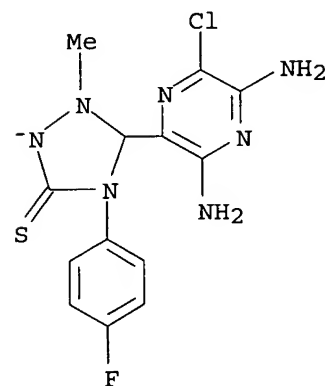
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2,4-dimethyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-14-4 HCAPLUS

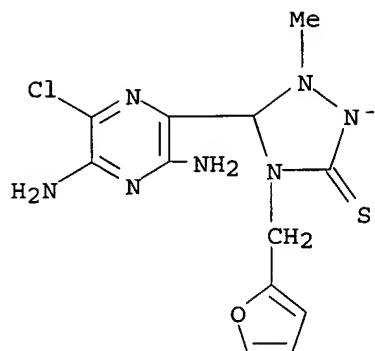
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4-(4-fluorophenyl)-4,5-dihydro-1-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-15-5 HCAPLUS

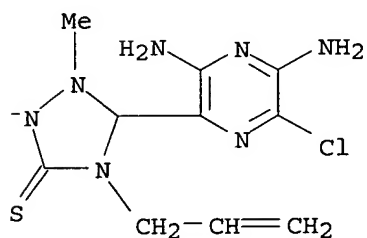
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2-methyl-4-phenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 80364-56-3 HCAPLUS

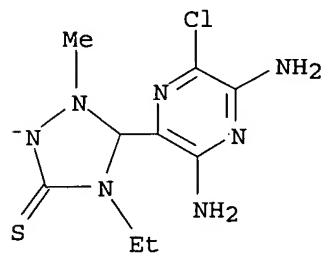
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2-methyl-4-(2-propenyl)-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 80377-35-1 HCAPLUS

CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4-ethyl-4,5-dihydro-2-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L22 ANSWER 31 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

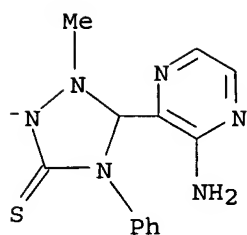
ACCESSION NUMBER: 1981:619467 HCAPLUS

DOCUMENT NUMBER: 95:219467

TITLE: <sup>13</sup>C-NMR spectra of anhydro-3-mercapto-5-pyrazinyl-1,2,4-triazolium hydroxides

AUTHOR(S): Shutske, Gregory M.; Agnew, Marc N.

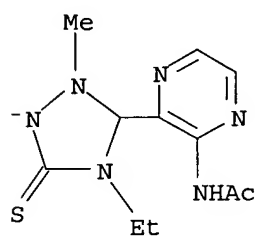
CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc.,



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-08-6 HCAPLUS

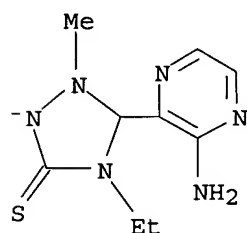
CN 1H-1,2,4-Triazolium, 3-[3-(acetylamino)pyrazinyl]-4-ethyl-4,5-dihydro-2-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-09-7 HCAPLUS

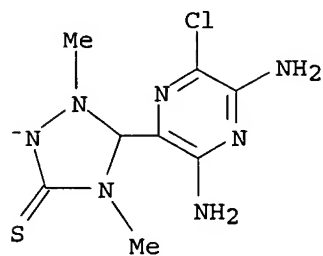
CN 1H-1,2,4-Triazolium, 3-(3-aminopyrazinyl)-4-ethyl-4,5-dihydro-2-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

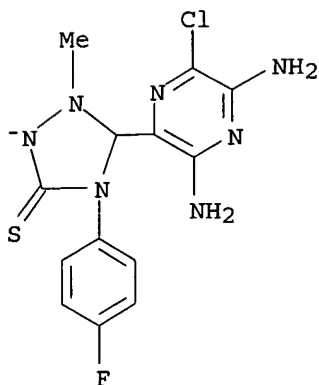


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-10-0 HCAPLUS

CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2,4-dimethyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

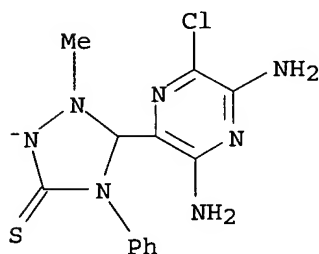




ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-15-5 HCAPLUS

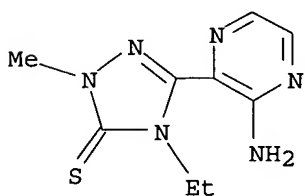
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2-methyl-4-phenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 79998-18-8 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(3-aminopyrazinyl)-4-ethyl-2,4-dihydro-2-methyl- (9CI) (CA INDEX NAME)

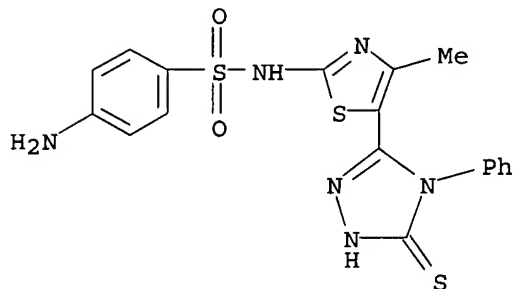


RN 79998-19-9 HCAPLUS

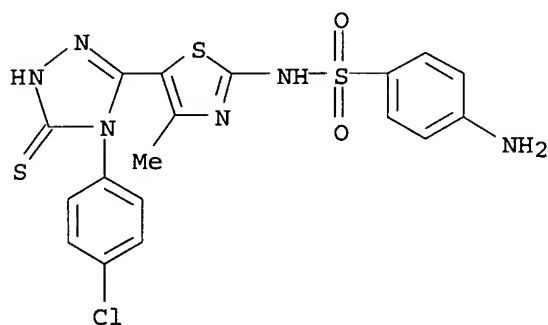
CN 3H-1,2,4-Triazole-3-thione, 5-(3-aminopyrazinyl)-2,4-dihydro-2-methyl-4-phenyl- (9CI) (CA INDEX NAME)



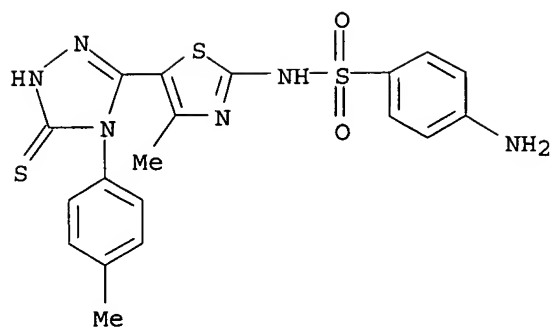
(X = O, S) resp. II (R = 4-ClC<sub>6</sub>H<sub>4</sub>) showed fungicidal activity at 200 ppm.  
 IT 78634-02-3P 78634-06-7P 78634-07-8P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation and fungicidal activity of)  
 RN 78634-02-3 HCAPLUS  
 CN Benzenesulfonamide, 4-amino-N-[5-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



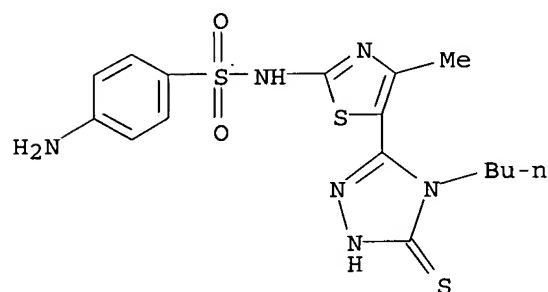
RN 78634-06-7 HCAPLUS  
 CN Benzenesulfonamide, 4-amino-N-[5-[4-(4-chlorophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl]-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 78634-07-8 HCAPLUS  
 CN Benzenesulfonamide, 4-amino-N-[5-[4,5-dihydro-4-(4-methoxyphenyl)-5-thioxo-1H-1,2,4-triazol-3-yl]-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 78634-08-9 HCAPLUS  
 CN Benzenesulfonamide, 4-amino-N-[5-(4-butyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



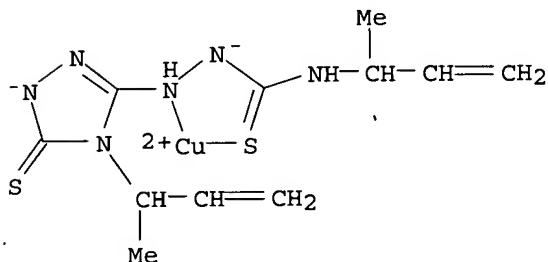
L22 ANSWER 33 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1979:540850 HCAPLUS  
 DOCUMENT NUMBER: 91:140850  
 TITLE: 1-(3-Mercapto-4-substituted-1,2,4-triazol-5-yl)-4-substituted-3-thiosemicarbazides  
 INVENTOR(S): Eberhardt, Udo; Depner, Johannes; Stopsack, Heinz; Oettel, Michael; Huebler, Doris; Chemnitius, Klaus Henning  
 PATENT ASSIGNEE(S): Ger. Dem. Rep.  
 SOURCE: Ger. (East), 20 pp.  
 CODEN: GEXXA8  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 133436	Z	19790103	DD 1977-201692	19771026 <--
PRIORITY APPLN. INFO.: GI			DD 1977-201692	A1 19771026

RN 71003-46-8 HCAPLUS  
 CN Copper, [2-[4,5-dihydro-4-(1-methyl-2-propenyl)-5-thioxo-1H-1,2,4-triazol-3-yl]-N-(1-methyl-2-propenyl)hydrazinecarbothioamidato(2-)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

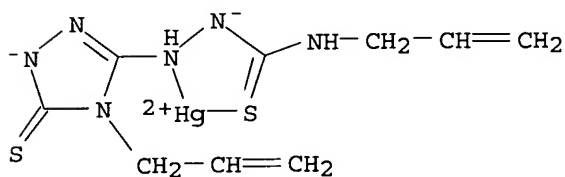
CRN 71003-45-7  
 CMF C11 H16 Cu N6 S2  
 CCI CCS



RN 71035-18-2 HCAPLUS  
 CN Mercury, [2-[4,5-dihydro-4-(2-propenyl)-5-thioxo-1H-1,2,4-triazol-3-yl]-N-2-propenylhydrazinecarbothioamidato(2-)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

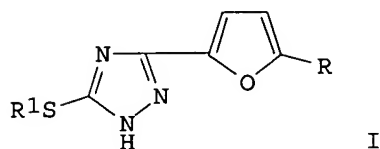
CRN 71035-17-1  
 CMF C9 H12 Hg N6 S2  
 CCI CCS



L22 ANSWER 34 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1977:502330 HCAPLUS  
 DOCUMENT NUMBER: 87:102330  
 TITLE: Substituted 5-nitroimidazoles  
 INVENTOR(S): Asato, Goro; Berkelhammer, Gerald; Gastrock, William Henry  
 PATENT ASSIGNEE(S): American Cyanamid Co., USA  
 SOURCE: U.S., 11 pp. Division of U.S. 3,940,411.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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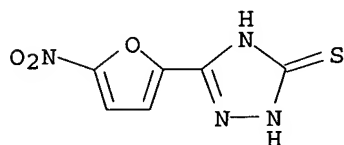
DOCUMENT TYPE: Conference  
 LANGUAGE: Russian  
 GI



AB Nitration of I (R = R1 = H) (II) with HNO<sub>3</sub>-Ac<sub>2</sub>O gave I (R = NO<sub>2</sub>, R1 = H). Treatment of II with furfuryl chloride gave I (R = H, R1 = furfuryl) which was nitrated to give I (R = NO<sub>2</sub>, R1 = nitrofurfuryl).

IT 57672-16-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with furfuryl chloride)

RN 57672-16-9 HCAPLUS  
 CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-5-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 36 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:29722 HCAPLUS  
 DOCUMENT NUMBER: 86:29722  
 TITLE: Nitrofuranyl heterocycles. XIII.  
 N-Methyl-3-methylthio-5-(5-nitro-2-furanyl)-1H-1,2,4-triazoles

AUTHOR(S): Benjamin, Louis E.; Snyder, Harry R., Jr.  
 CORPORATE SOURCE: Norwich Pharmacal Co. Div., Morton-Norwich Prod., Inc., Norwich, NY, USA

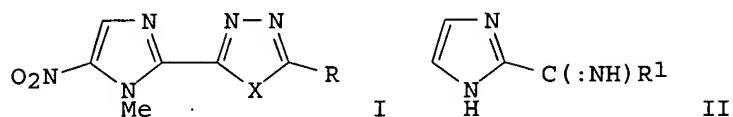
SOURCE: Journal of Heterocyclic Chemistry (1976), 13(5), 1115-18  
 CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3940411	A	19760224	US 1973-409505	19731025 <--
US 3649638	A	19720314	US 1969-863378	19691002 <--
AT 292692	B	19710910	AT 1969-9579	19691010 <--
FR 2020451	A5	19700710	FR 1969-35003	19691013 <--
FR 2020451	B1	19740111		
US 3790589	A	19740205	US 1971-202568	19711126 <--
US 4026903	A	19770531	US 1975-632941	19751118 <--
PRIORITY APPLN. INFO.:			US 1968-766984	A2 19681011
			US 1969-863378	A3 19691002
			US 1971-202568	A3 19711126
			US 1973-409505	A3 19731025

GI



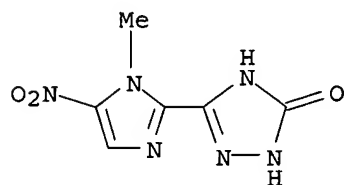
AB The imidazoles I (R = Me, H<sub>2</sub>N, X = NH; R = H<sub>2</sub>N, X = O, S) were prepared. Thus, II (R<sub>1</sub> = EtO) was treated with MeCONHNH<sub>2</sub> to give II (R = MeCONHNH), which was cyclized with HOAc to give I (R = Me, X = NH) (III). At 160 mg/kg I (R = H<sub>2</sub>N, X = S) cured pullet chicks infected with *Escherichia coli*. At 200 mg/kg III cleared mice infected with *Trichomonas vaginalis*.

IT 27344-17-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 27344-17-8 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 1,2-dihydro-5-(1-methyl-5-nitro-1H-imidazol-2-yl)-  
 (9CI) (CA INDEX NAME)



L22 ANSWER 38 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:4868 HCAPLUS

DOCUMENT NUMBER: 84:4868

TITLE: 1,2,4-Triazole derivatives

AUTHOR(S): Lipanova, M. D.; Burov, E. V.; Kulikova, L. K.

CORPORATE SOURCE: USSR

SOURCE: Issled. V Obl. Sintezy I Kataliza Organ. Soedinenii (  
 1975) 29

From: Ref. Zh., Khim. 1975, Abstr. No. 16ZH259

DOCUMENT TYPE: Journal

group which can be accommodated at C5 without a complete loss of activity. All of the 5-membered heterocyclic rings showed some activity. Activity was highest when the ring was nonarom. and a 5-membered nonarom. ring was more active than a 6-membered nonarom. ring. None of these derivs. were as active as the compds. with smaller nonannulated groups at position 5.

IT 55470-38-7P

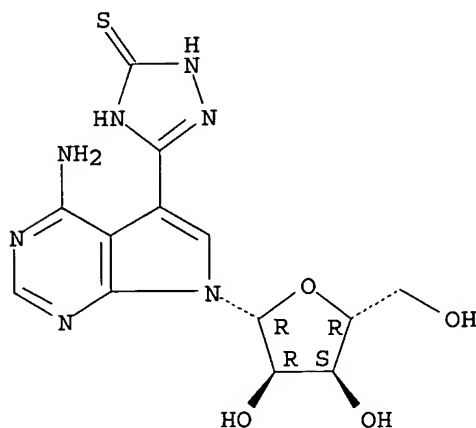
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and neoplasm inhibiting activity of)

RN 55470-38-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(4-amino-7-β-D-ribofuranosyl-7H-pyrrolo[2,3-d]pyrimidin-5-yl)-1,2-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 40 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:563330 HCAPLUS

DOCUMENT NUMBER: 81:163330

TITLE: Nitrofurans with high renal excretion

AUTHOR(S): Akerblom, Eva B.

CORPORATE SOURCE: Dep. Org. Chem., Pharm. AB, Uppsala, Swed.

SOURCE: Journal of Medicinal Chemistry (1974), 17(7), 756-8

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Of the 16 title compds. tested, those with acidic groups were prepared by reaction of Et haloacetate with the Na salt of the appropriate nitrofurans compound, while those with the nitroamino group were prepared by nitration of the corresponding amino compds. The in vitro antibacterial activity of the new compds. was low, with the esters showing more activity than the acids. Against Trichomonas vaginalis, the esters I [52980-64-0] and II [27550-27-2] show very high activity. II [52980-53-7] and IV [52980-65-1], tested for peroral absorption and urinary excretion in dogs, were >60% recovered in the urine. Urinary excretion was blocked by probenidicid, indicating tubular excretion.

IT 52980-62-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(alkylation of)

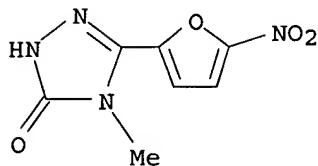
RN 52980-62-8 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-methyl-5-(5-nitro-2-furanyl)-,

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and bactericidal activity of)

RN 41735-59-5 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-methyl-5-(5-nitro-2-furanyl)- (9CI)  
(CA INDEX NAME)



L22 ANSWER 42 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:564610 HCAPLUS

DOCUMENT NUMBER: 77:164610

TITLE: Reactions of 3-hydrazino-1,2,4-triazoles with dicyandiamide

AUTHOR(S): Uteg, Karl Heinz

CORPORATE SOURCE: Bezirksinst. Blutspende- Transfusionswes., Schwerin, Ger. Dem. Rep.

SOURCE: Zeitschrift fuer Chemie (1972), 12(8), 291

CODEN: ZECEAL; ISSN: 0044-2402

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

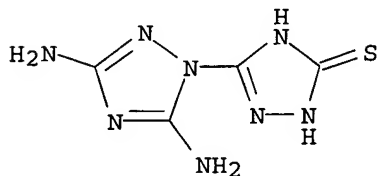
AB Refluxing the triazoles (I, R = H, SH, Ph, o-ClC<sub>6</sub>H<sub>4</sub>, o-MeOC<sub>6</sub>H<sub>4</sub>, o-, m-, p-MeC<sub>6</sub>H<sub>4</sub>) with H<sub>2</sub>NC(:NH)NHCN in HCl-H<sub>2</sub>O yielded 36-68 guanazoles (II). Uv spectroscopic data of II were reported.

IT 38767-47-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 38767-47-4 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(3,5-diamino-1H-1,2,4-triazol-1-yl)- (9CI)  
(CA INDEX NAME)



L22 ANSWER 43 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

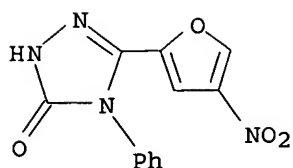
ACCESSION NUMBER: 1972:526568 HCAPLUS

DOCUMENT NUMBER: 77:126568

TITLE: Synthesis of pyrazine derivatives as potential hypoglycemic agents

AUTHOR(S): Ambrogi, V.; Bloch, K.; Daturi, S.; Logemann, W.; Parenti, M. A.

CORPORATE SOURCE: Antidiabetic Dep., Carlo Erba Res. Inst., Milan, Italy



L22 ANSWER 45 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:425480 HCAPLUS  
 DOCUMENT NUMBER: 73:25480  
 TITLE: 1,2-Disubstituted 5-nitroimidazoles  
 INVENTOR(S): Asato, Goro; Berkelhammer, Gerald; Gastrock, William H.; Starer, Ira; Papaioamiou, Christos G.; Albright, Jay D.; Shepherd, Robert G.  
 PATENT ASSIGNEE(S): American Cyanamid Co.  
 SOURCE: Ger. Offen., 44 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1951259	A	19700527	DE 1969-1951259	19691010 <--
US 3652555	A	19720328	US 1969-833683	19690616 <--
AT 292692	B	19710910	AT 1969-9579	19691010 <--
FR 2020451	A5	19700710	FR 1969-35003	19691013 <--
FR 2020451	B1	19740111		
PRIORITY APPLN. INFO.:			US 1968-766984	A 19681011
			US 1969-833683	A 19690616

GI For diagram(s), see printed CA Issue.

AB The title compds. (I and II), active against chicken typhus, enteritis, colibacillosis, and Trichomonas vaginalis, were prepared I (X = NH) were prepared by treatment of the corresponding Et 5-nitroimidazole-2-carboximidates, obtained from 5-nitro-2-cyanoimidazoles (III), with acylhydrazines, H<sub>2</sub>NNHC(:NH)NH<sub>2</sub>, H<sub>2</sub>NNHCONH<sub>2</sub>, or H<sub>2</sub>NNHCSNH<sub>2</sub>. Reaction of the corresponding 5-nitro-2-(chloroformyl)imidazoles with H<sub>2</sub>NNHCONH<sub>2</sub> or H<sub>2</sub>NNHCSNH<sub>2</sub> gave I (X = O). The following I were prepared (R, R<sub>1</sub>, and X given): Me, Ac, NH (Ia); Me, C(:NH)NH<sub>2</sub>, NH; Me, CONH<sub>2</sub>, NH; Me, CSNH<sub>2</sub>, NH; Me, CSNH<sub>2</sub>, O; HOCH<sub>2</sub>CH<sub>2</sub>, CSNH<sub>2</sub>, O; Me, CONH<sub>2</sub>, O; AcOCH<sub>2</sub>CH<sub>2</sub>, CSNH<sub>2</sub>, NH; and BzOCH<sub>2</sub>CH<sub>2</sub>, CSNH<sub>2</sub>, NH. Cyclization of I gave the following II (R, R<sub>2</sub>, and Y given): Me, Me, NH; Me, NH<sub>2</sub>, NH; Me, NH<sub>2</sub>, S (IIa); Me, NH<sub>2</sub>, O; BzOCH<sub>2</sub>CH<sub>2</sub>, NH<sub>2</sub>, S; and HOCH<sub>2</sub>CH<sub>2</sub>, NH<sub>2</sub>, S. II (Y = S) were also directly obtained from III by treating III with H<sub>2</sub>NNHCSNH<sub>2</sub> in the absence of H<sub>2</sub>O and in the presence of a strong acid. Chickens, infected with chicken typhus, were treated with food containing 0.1% Ia or 0.05% IIa. Of 5 chickens all survived, whereas of 20 untreated chickens all died.

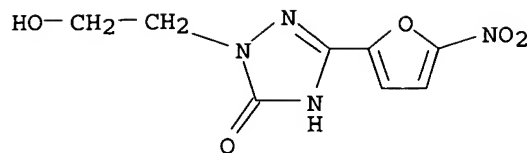
IT 27344-17-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

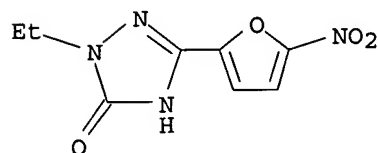
RN 27344-17-8 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 1,2-dihydro-5-(1-methyl-5-nitro-1H-imidazol-2-yl)-  
 (9CI) (CA INDEX NAME)

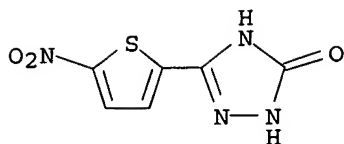




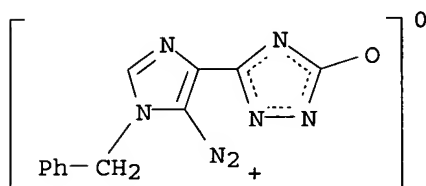
RN 25142-90-9 HCAPLUS  
 CN 3H-1,2,4-Triazol-3-one, 2-ethyl-2,4-dihydro-5-(5-nitro-2-furanyl) - (9CI)  
 (CA INDEX NAME)



L22 ANSWER 47 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1969:106436 HCAPLUS  
 DOCUMENT NUMBER: 70:106436  
 TITLE: Heteroaromaticity. XX. Novel thermal 1,3-dipolar cycloaddition of 5-nitrofuran-2-carbohydroxamoyl chloride with diketene and dicyclohexylcarbodiimide  
 AUTHOR(S): Sasaki, Tadashi; Yoshioka, Toshiyuki  
 CORPORATE SOURCE: Nagoya Univ., Nagoya, Japan  
 SOURCE: Bulletin of the Chemical Society of Japan ( 1969), 42(1), 258-60  
 CODEN: BCSJA8; ISSN: 0009-2673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 5-Nitrofuran-2-carbohydroxamoyl chloride (I) was heated in toluene with diketene until the evolution of HCl stopped. Spectral data and elemental anal. confirmed that the product was 3-(5-nitro-2-furyl)-5-methylisoxazole, m. 143-4°. I was heated in toluene with an equivalent amount of dicyclohexylcarbodiimide (II) until the evolution of HCl ceased. After removal of the solvent under reduced pressure, the residue was dissolved in CHCl<sub>3</sub> and chromatographed on a silica gel column to give 1,4-dicyclohexyl-3-(5-nitro-2-furyl)-4,5-dihydro-5-oxo-1H-triazole (III). When an ethanolic solution of III was refluxed with EtONa, 1,3-dicyclohexylurea was recovered. Thermal treatment of 5-nitrofuran-2-carboxaldehyde oxime with II and the normal treatment of 5-nitrofuran-2-carbonitrile oxide with II in ether at room temperature both gave 5-nitrofuran-2-carbonitrile and no cyclization occurred. Possible reaction mechanisms were discussed.  
 IT 22200-72-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 22200-72-2 HCAPLUS  
 CN Δ2-1,2,4-Triazolin-5-one, 1,4-dicyclohexyl-3-(5-nitro-2-furyl) - (8CI) (CA INDEX NAME)



L22 ANSWER 49 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1967:443155 HCAPLUS  
 DOCUMENT NUMBER: 67:43155  
 TITLE: Diazo- $\beta$ -azomethine-v-triazine equilibrium  
 AUTHOR(S): Temple, Carroll, Jr.; Kussner, Conrad L.; Montgomery, John A.  
 CORPORATE SOURCE: Kettering-Meyer Lab., Southern Res. Inst., Birmingham, AL, USA  
 SOURCE: Journal of Organic Chemistry (1967), 32(7), 2241-5  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The nitrosation of some 3-[5- (or 4-)aminoimidazol-4-(or 5-)-yl]-s-triazoles and 5-[5- (or 4-)-aminoimidazole-4- (or 5-)-yl]tetrazoles is described. The resulting diazoimidazole-v-triazine systems are used to study the effect of solvent and certain groups on the diazo- $\beta$ -azomethine-v-triazine equilibrium Structure assignments are based on data obtained from the ir and proton N.M.R. spectra. 10 references.  
 IT 12129-55-4P 13976-26-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 12129-55-4 HCAPLUS  
 CN Imidazole-5-diazonium, 1-benzyl-4-(5-hydroxy-s-triazol-3-yl)-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 13976-26-6 HCAPLUS  
 CN s-Triazol-3-ol, 5-(5-amino-1-benzylimidazol-4-yl)-, monohydrochloride (8CI) (CA INDEX NAME)

AB New substituted nitrofuryltriazoines, I, where R can be H, Me, Ac, CH<sub>2</sub>CH<sub>2</sub>OH, or diethoxythiophosphoryl, and R<sub>1</sub> can be O, imino (substituted or not), or acetylmino, are used as antiseptics and antiparasitics. Dry HCl is passed through a cooled mixture of 900 g. 5-nitro-2-furonitrile and 5450 cc. anhydrous EtOH for 3.5-4.5 hrs. The solid is filtered off, washed with 150 cc. EtOH, and anhydrous Et<sub>2</sub>O to give 808 g. ethyl 5-nitro-2-furimidate-HCl (II), m. 158-60°. A mixture of 100 g. II, 84 g. semicarbazide, and 300 cc. EtOH is heated at 50-5° 30 min. with stirring, cooled, and diluted with 2000 cc. water. The product is filtered off to give 60 g. 5-nitro-2-furamide-N-ureide (III), m. 274-5°. A solution of 60 g. III in 450 cc. nitrobenzene is refluxed 15 min., cooled, and diluted with 400 cc. Et<sub>2</sub>O. The solid is filtered off, washed with Et<sub>2</sub>O, and crystallized (water) to give 31 g. 5-oxo-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline, m. 277-9°. II (110 g.) is added to a solution of 55 g. aminoguanidine-HCl in 600 cc. HCONMe<sub>2</sub>. The solution is heated at 50-60° 30 min., cooled, and diluted with Et<sub>2</sub>O. The oily solid is washed with EtOH and Et<sub>2</sub>O, and dried to give 90 g. 5-nitro-2-furamide-N-guanidine-2HCl (IV), m. 204-5°. A solution of 90 g. IV in 400 cc. nitrobenzene is refluxed 15 min., filtered, cooled, and diluted with Et<sub>2</sub>O. The solid is filtered off, washed with Et<sub>2</sub>O and dried to give 32 g. 5-imino-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline (V), m. 289-90° (H<sub>2</sub>O). A mixture of 110 g. II, 45 g. 2-methylsemicarbazide, and 500 cc. EtOH is heated at 50-60° 1 hr., cooled, and diluted with Et<sub>2</sub>O. The solid is filtered off to give 100 g. 5-nitro-2-furamide-N-(1-methylureide)-HCl (VI), which is treated with Na<sub>2</sub>CO<sub>3</sub> to give 5-nitro-2-furamide-N-(1-methylureide), m. 185-6°. A solution of 100 g. VI in 400 cc. nitrobenzene is refluxed 15 min., cooled, and diluted with Et<sub>2</sub>O. The solid is filtered off, and washed with Et<sub>2</sub>O, to give 35 g. 1-methyl-5-oxo-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline, m. 275-6° (H<sub>2</sub>O). A mixture of 20 g. V, 10 cc. Ac<sub>2</sub>O, and 300 cc. anhydrous AcOH is heated on a water bath for 20 min., cooled, and diluted with Et<sub>2</sub>O. The solid is filtered off and crystallized (HCONMe<sub>2</sub>-water) to give 30 g. 1-acetyl-5-imino-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline (VII). Dry HCl (5.5 g.) is introduced into a solution of 29 g. V in 580 cc. anhydrous

AcOH.

The solution is heated 20 hrs., cooled, and diluted with water. The solid is filtered off to give 25 g. 5-acetylmino-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline (VIII), m. 343-5° (HCONMe<sub>2</sub>). VII (4.8 g.) is added with stirring to 20 g. benzophenone at 290°. The mixture is heated at 290-5° 2 min., cooled, and diluted with Et<sub>2</sub>O, and the solid filtered off to give VIII, m. 343-5° (HCONMe<sub>2</sub>). A mixture of 24 g. II, 24 g. 2-(2-hydroxyethyl)semicarbazide, and 300 cc. EtOH is heated at 50-60° 30 min., cooled, and diluted with Et<sub>2</sub>O. The solid is filtered off, and dissolved in water. This solution is filtered, alkalized with Na<sub>2</sub>CO<sub>3</sub>, cooled, and the solid filtered off to give 20 g. 5-nitro-2-furamide-N-[1-(2-hydroxyethyl)ureide], m. 175-80°, which treated with dry HCl in a suitable solvent gives 5-nitro-2-furamide-N-[1-(2-hydroxyethyl)ureide]-HCl (IX). A mixture of 144 g. IX and 400 cc. nitrobenzene is refluxed 15 min., filtered, cooled, and diluted with Et<sub>2</sub>O. The solid is filtered off and washed with 50% AcOH to give 45 g. 1-(2-hydroxyethyl)-5-oxo-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline, m. 263-4° (AcOH). A mixture of 58.5 g. V, 56.7 g. diethylthionophosphoryl chloride, 16.2 g. NaOMe, and 1200 cc. EtOH is refluxed 30 min., filtered, cooled, and diluted with water. The solid is filtered off to give 29 g. 1-(O,O-diethyl thiophosphate)-5-imino-3-(5-nitro-2-furyl)-Δ<sup>2</sup>-1,2,4-triazoline, m. 160-1° (MeOH). A solution of 37.2 g. 1-amino-1-methylguanidine-HCl, and 66.3 g. II in 300 cc. HCONMe<sub>2</sub> is heated at 50-60° 30 min., cooled, and diluted with Et<sub>2</sub>O. The gummy precipitate is washed with Et<sub>2</sub>O, and dried to give

5-nitro-2-furamide-

Lambkin 10\_678331

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